

# Coulomb matrix elements in multi-orbital Hubbard models

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**Abstract.** Coulomb matrix elements are needed in all studies in solid-state theory that are based on Hubbard-type multi-orbital models. Due to symmetries, the matrix elements are not independent. We determine a set of independent Coulomb parameters for a  $d$ -shell and an  $f$ -shell and all point groups with up to 16 elements ( $O_h$ ,  $O$ ,  $T_d$ ,  $T_h$ ,  $D_{6h}$ , and  $D_{4h}$ ). Furthermore, we express all other matrix elements as a function of the independent Coulomb parameters. Apart from the solution of the general point-group problem we investigate in detail the spherical approximation and first-order corrections to the spherical approximation.

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## 1. Introduction

One of the main weaknesses of state-of-the-art band-structure methods is their frequent failure to describe the electronic properties of systems with partially filled  $d$ -shells or  $f$ -shells. The orbitals of such shells are well localised which often leads to substantial correlation effects. These effects are not captured by effective single-particle approaches such as the common methods based on Density-Functional Theory (DFT). Over the past 15 years it has therefore been a general trend to combine ab-initio methods with many-particle approaches that permit a more sophisticated treatment of local correlations.

To this end, one usually separates the two-particle interactions into non-local and local terms. While the former are treated in the standard (e.g., DFT) way, the latter are studied by means of many-particle methods such as Dynamical Mean Field Theory [1] or the variational Gutzwiller approach [2, 3]. In general, the local Coulomb interaction ('Hubbard interaction') has the form

$$\hat{H}_C = \sum_i \sum_{\substack{b_1, b_2 \\ b_3, b_4}} U_{b_1, b_2, b_3, b_4}^i \sum_{\sigma, \sigma'} \hat{c}_{i, b_1, \sigma}^\dagger \hat{c}_{i, b_2, \sigma'}^\dagger \hat{c}_{i, b_3, \sigma'} \hat{c}_{i, b_4, \sigma}, \quad (1)$$

where  $i$ ,  $b_l$ , and  $\sigma, \sigma'$  denote the lattice site, (correlated) orbital indices, and spin indices, respectively. Depending on the number  $n_o$  of correlated orbitals per site, there can be up to  $n_o^4$  non-zero Coulomb-interaction parameters  $U_{b_1, b_2, b_3, b_4}^i$ . In most cases, however, this number is much smaller due to the point-group symmetry at the lattice site  $i$ . Moreover, the non-zero parameters are not independent, but can be expressed by a sub-set of independent parameters.

It is the purpose of this work to analyse in detail which Coulomb matrix elements vanish due to symmetry and which of them are independent for all high-symmetry point groups in the most relevant cases of a  $d$ -shell or an  $f$ -shell. Note that the lattice-site index  $i$  enters the problem only through its point-group symmetry and will therefore be dropped in our following considerations.

The special case of a  $d$ -shell in a cubic environment was analysed in the textbook by Sugano, Tanabe, and Kamimura [4]. In contrast to our approach, however, their method cannot be readily applied to other systems. To reduce the number of independent parameters, one often employs the 'spherical approximation', in which the matrix elements are calculated with atomic wave functions, i.e., without a crystal field [5, 6, 7]. We shall derive the spherical approximation in a different way by using the same method that we develop for the full point-group problem. This enables us to formulate also a systematic first-order correction to the spherical approximation.

In solids we often face the situation that not all of the  $d$ -orbitals or the  $f$ -orbitals are partially filled. In such cases, only the sub-sets of partially filled orbitals must be included in the Hubbard interaction (1). Note that the general results which we present in this work can be readily applied in all these cases as well. One just needs to drop all those matrix elements which contain orbitals that are not taken into account in (1).

Our work is organised as follows. In section 2 we develop the general approach for the analysis of Coulomb matrix elements which is used throughout this work. The appropriate orbital basis for a  $d$ -shell and an  $f$ -shell are introduced in section 3. In the following sections 4, 5, and 6, we analyse the Coulomb matrix elements for, (i) the full point group, (ii), the spherical approximation, and, (iii), a first-order correction to the spherical approximation, respectively. A summary, in section 7, closes our presentation. Most of the explicit results are deferred to four appendices.

## 2. General formalism

Depending on the point-group symmetry at the site of a correlated atom in a lattice, the  $n_o = 5$   $d$ -orbitals or  $n_o = 7$   $f$ -orbitals split up into orbitals  $\varphi_b(\mathbf{r})$  ( $b = 1, \dots, n_o$ ) with a maximally three-fold degeneracy. Each orbital belongs to an irreducible representation  $\Gamma^p$  of the point group  $G^{\text{point}}$  at the transition-metal site. The occurring representations  $\Gamma^p$  are obtained from a reduction of the  $j = 2$  and  $j = 3$  representations  $\Gamma^j$  of the full rotational group  $O(3)$ ,

$$\Gamma^j = \sum_p n_p^j \Gamma^p. \quad (2)$$

We will introduce the coefficients  $n_p^j$  for all relevant point groups in section 3.

Without spin-orbit coupling, the orbitals  $\varphi_b(\mathbf{r})$  can be represented by real wave functions. The  $g$  point group operations, described by three-dimensional orthogonal matrices  $\tilde{D}_l$  ( $l = 1, \dots, g$ ), have isomorph unitary operators  $\hat{T}_l$  in the Hilbert space, defined by

$$\hat{T}_l \Psi(\mathbf{r}) = \Psi(\tilde{D}_l \mathbf{r}). \quad (3)$$

Note that, when applied to many-particle wave functions, the operator transforms all spatial coordinates simultaneously,

$$\hat{T}_l \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \Psi(\tilde{D}_l \mathbf{r}_1, \dots, \tilde{D}_l \mathbf{r}_N). \quad (4)$$

The behaviour of orbital wave functions under point-group transformations is well defined,

$$\hat{T}_l \varphi_b(\mathbf{r}) = \sum_{b'} \Gamma_{b', b}^p(l) \varphi_{b'}(\mathbf{r}), \quad (5)$$

where  $\Gamma_{b', b}^p(l)$  denote the elements of the irreducible representation matrices  $\tilde{\Gamma}^p(l)$ . These matrices are documented for all 32 crystallographic point groups in

the literature, see, e.g., Ref. [8]. In the following we drop the label  $p$  in  $\Gamma_{b',b}^p(l)$  because its information is already included in the orbital indices  $b, b'$ .

To set up the local Hamiltonian (1), we need to determine the  $D_d = 5^4 = 625$  (or  $D_f = 7^4 = 2401$ ) Coulomb matrix elements

$$U_{b_1, b_2, b_3, b_4} \quad (6)$$

$$= \int d^3r \int d^3r' \varphi_{b_1}(\mathbf{r}) \varphi_{b_2}(\mathbf{r}') f(\mathbf{r}, \mathbf{r}') \varphi_{b_3}(\mathbf{r}') \varphi_{b_4}(\mathbf{r}),$$

where  $f(\mathbf{r}, \mathbf{r}')$  is the screened Coulomb interaction. The exact form of this interaction is usually not known, however, our analysis only requires that it is invariant under all transformations of the respective point group. When we insert  $\hat{1} = \hat{T}_l^\dagger \hat{T}_l$  on the left-hand-side and on the right-hand-side of  $f(\mathbf{r}, \mathbf{r}')$  in (6) and use

$$[\hat{T}_l, f(\mathbf{r}, \mathbf{r}')]_- = 0, \quad (7)$$

we find

$$U_{b_1, \dots, b_4} = \sum_{\bar{b}_1, \dots, \bar{b}_4} \Gamma_{\bar{b}_1, b_1}(l) \dots \Gamma_{\bar{b}_4, b_4}(l) U_{\bar{b}_1, \dots, \bar{b}_4}. \quad (8)$$

With the multiple index

$$\mathbf{B} = (b_1, \dots, b_4) \quad (9)$$

and the vectors  $\mathbf{U}$  with components  $U_{\mathbf{B}}$ , equations (8) assume the compact form

$$\mathbf{U} = \tilde{\Gamma}(l) \cdot \mathbf{U} \quad (l = 1, \dots, g). \quad (10)$$

Here we introduced the product matrices  $\tilde{\Gamma}(l)$  with the elements

$$\Gamma_{\mathbf{B}, \mathbf{B}}(l) = \Gamma_{(\bar{b}_1, \dots, \bar{b}_4), (b_1, \dots, b_4)}(l) \quad (11)$$

$$= \Gamma_{\bar{b}_1, b_1}(l) \dots \Gamma_{\bar{b}_4, b_4}(l). \quad (12)$$

Equation (10) shows that we need to calculate the space of joint eigenvectors of all  $g$  matrices  $\tilde{\Gamma}(l)$  with the same eigenvalue  $\lambda = 1$ . Suppose we have found a  $d$ -dimensional (orthogonal and normalised) basis  $\mathbf{c}^{(k)}$  ( $k = 1, \dots, d$ ) of this space and a basis  $\mathbf{d}^{(k')}$  ( $k' = 1, \dots, D-d$ ) of its orthogonal complement. Then, since all matrices  $\tilde{\Gamma}(l)$  are regular, equation (10) leads to

$$I^k = \sum_{\mathbf{B}} c_{\mathbf{B}}^{(k)} U_{\mathbf{B}}, \quad (13)$$

$$0 = \sum_{\mathbf{B}} d_{\mathbf{B}}^{(k')} U_{\mathbf{B}}, \quad (14)$$

where we introduced  $d$  independent Coulomb parameters  $I^k$ . A simple inversion of these equations gives us all Coulomb matrix elements  $U_{\mathbf{B}}$  as a function of the independent parameters  $I^k$ . Since any rotation of the vectors  $\mathbf{c}^{(k)}$  is permitted there is a freedom in the choice of the parameters  $I^k$ . We shall find it most convenient to chose them as a set of  $d$  independent matrix elements  $U_{\mathbf{B}}^{(i)}$ , see section 4.

The number  $d$  of independent matrix elements can be determined by the following group-theoretical

considerations without a complete solution of equations (10). The matrices  $\tilde{\Gamma}(l)$  define the product representation of four irreducible representations  $\Gamma^j$ ,

$$\Gamma = \Gamma^j \otimes \Gamma^j \otimes \Gamma^j \otimes \Gamma^j. \quad (15)$$

With (2) this equation reads

$$\Gamma = \sum_{p_1, p_2, p_3, p_4} n_{p_1}^j n_{p_2}^j n_{p_3}^j n_{p_4}^j \Gamma^{p_1, p_2, p_3, p_4}, \quad (16)$$

$$\Gamma^{p_1, p_2, p_3, p_4} \equiv \Gamma^{p_1} \otimes \Gamma^{p_2} \otimes \Gamma^{p_3} \otimes \Gamma^{p_4}. \quad (17)$$

The reduction of (17) into irreducible components can be derived from the multiplication tables for the point groups [8]. For example, in cubic symmetry, there is one contribution in (16) with all  $p_i$  belonging to an  $E_g$  representation. Its reduction is given as

$$\Gamma^{E_g, E_g, E_g, E_g} = 3\Gamma^{A_{1g}} + 3\Gamma^{A_{2g}} + 5\Gamma^{E_g}. \quad (18)$$

In this way we can determine all coefficients in the reduction of  $\Gamma$ ,

$$\Gamma = \sum_p n(p) \Gamma^p. \quad (19)$$

To find the joint eigenvectors to the eigenvalue  $\lambda = 1$  in (10) is mathematically equivalent to the determination of the space that belongs to the totally symmetric representation  $A_{1g}$  on the right hand side of (19). Its dimension  $n(A_{1g})$  is just the number  $d$  of independent Coulomb matrix elements  $I^k$ . For example, we can conclude from (18) that in a pure  $E_g$  shell there would be three such parameters. Alternatively, we can calculate  $n(A_{1g})$  with the general formula [9]

$$n(p) = \frac{1}{g} \sum_l (\chi(l))^* \chi^p(l) \quad (20)$$

for the coefficients in (19) where  $\chi(l)$ ,  $\chi^p(l)$  are the characters of  $\Gamma$ ,  $\Gamma^p$ , respectively. For  $p = A_{1g}$  (i.e.,  $\chi^p(l) = 1$ ) this equation reads

$$d = n(A_{1g}) = \frac{1}{g} \sum_l \sum_{\mathbf{B}} \Gamma_{\mathbf{B}, \mathbf{B}}(l). \quad (21)$$

Thus far, we only made use of the commutator relation (7) and of the transformation behaviour (5) of the orbitals. Hence, our analysis applies to rather general matrix elements such as

$$U'_{b'_1, b_2, b_3, b_4} = \int d^3r_1 \int d^3r_2 \int d^3r_3 \int d^3r_4 \quad (22)$$

$$\varphi_{b'_1}^{p_1}(\mathbf{r}_1) \varphi_{b_2}^{p_2}(\mathbf{r}_2) f(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \varphi_{b_3}^{p_3}(\mathbf{r}_3) \varphi_{b_4}^{p_4}(\mathbf{r}_4),$$

as long as  $f(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4)$  commutes with all  $\hat{T}_l$ . Our physical Coulomb matrix elements (6), however, have the additional permutation symmetries

$$U_{b_1, b_2, b_3, b_4} = U_{b_1, b_3, b_2, b_4}, \quad (23)$$

$$U_{b_1, b_2, b_3, b_4} = U_{b_4, b_2, b_3, b_1}, \quad (24)$$

$$U_{b_1, b_2, b_3, b_4} = U_{b_3, b_1, b_4, b_2}. \quad (25)$$

These permutations define a group  $G^{\text{perm}}$  with the eight elements

$$\begin{aligned} (1, 2, 3, 4) &\rightarrow (1, 2, 3, 4) \equiv \hat{P}_1, \\ &\rightarrow (1, 3, 2, 4) \equiv \hat{P}_2, \\ &\rightarrow (4, 2, 3, 1) \equiv \hat{P}_3, \\ &\rightarrow (4, 3, 2, 1) \equiv \hat{P}_4, \\ &\rightarrow (2, 1, 4, 3) \equiv \hat{P}_5, \\ &\rightarrow (2, 4, 1, 3) \equiv \hat{P}_6, \\ &\rightarrow (3, 1, 4, 2) \equiv \hat{P}_7, \\ &\rightarrow (3, 4, 1, 2) \equiv \hat{P}_8, \end{aligned} \quad (26)$$

which is isomorph to the point group  $D_{2h}$ .

The matrices  $\tilde{P}(i)$  with the elements

$$\tilde{P}_{\mathbf{B}, \mathbf{B}'}(i) \equiv \langle \mathbf{B} | \hat{P}_i | \mathbf{B}' \rangle \quad (27)$$

form a  $D$ -dimensional representation of  $G^{\text{perm}}$ . The permutation symmetry of our Coulomb matrix elements can then be cast into the same form as in (10),

$$\mathbf{U} = \tilde{P}(i) \cdot \mathbf{U} \quad (i = 1, \dots, 8). \quad (28)$$

Therefore, we need to find the space of joint eigenvectors  $\mathbf{c}^{(k)}$  to the eigenvalue  $\lambda = 1$ , not only of the matrices  $\tilde{\Gamma}(l)$  but also of  $\tilde{P}(i)$ . The dimension of this space is smaller than that without the additional permutation symmetries. This reduces the number  $d$  of independent Coulomb parameters  $I^k$ . It can also be determined by group-theoretical arguments, i.e., without an explicit solution of equations (10), (28), as we explain in Appendix A.

### 3. Crystal-field splitting

In this work we study  $d$ -orbitals and  $f$ -orbitals in environments that are described by crystallographic point groups with up to 16 elements. These groups are  $O_h$ ,  $O$ ,  $T_d$ ,  $T_h$ ,  $D_{6h}$ , and  $D_{4h}$ . It turns out that the Coulomb integrals for the groups  $O_h$ ,  $O$  and  $T_d$  are the same. Hence, we only need to study four different cases.

As a starting point for our further considerations, we introduce the proper orbital basis states in all point-group environments. The situation is simplest for a  $d$ -shell since here we can set up irreducible spaces for all our point groups with the same basis,

$$\begin{aligned} \varphi_v(r, \varphi, \theta) &= \frac{1}{\sqrt{2}} R_v(r) [Y_{2,2}(\varphi, \theta) + Y_{2,-2}(\varphi, \theta)] \\ &\sim (x^2 - y^2), \end{aligned} \quad (29)$$

$$\varphi_u(r, \varphi, \theta) = R_u(r) Y_{2,0}(\varphi, \theta) \sim (3z^2 - r^2). \quad (30)$$

$$\begin{aligned} \varphi_\zeta(r, \varphi, \theta) &= -\frac{i}{\sqrt{2}} R_\zeta(r) [Y_{2,2}(\varphi, \theta) - Y_{2,-2}(\varphi, \theta)] \\ &\sim xy, \end{aligned} \quad (31)$$

$$\varphi_\eta(r, \varphi, \theta) = -\frac{1}{\sqrt{2}} R_\eta(r) [Y_{2,1}(\varphi, \theta) - Y_{2,-1}(\varphi, \theta)]$$

$$\sim xz, \quad (32)$$

$$\begin{aligned} \varphi_\xi(r, \varphi, \theta) &= \frac{i}{\sqrt{2}} R_\xi(r) [Y_{2,1}(\varphi, \theta) + Y_{2,-1}(\varphi, \theta)] \\ &\sim yz. \end{aligned} \quad (33)$$

Here, we introduced the ‘spherical harmonic’ functions  $Y_{l,m}(\varphi, \theta)$  ( $m = -l, \dots, l$ ) [10], and the unspecified radial wave functions  $R_b(r)$ . Note that, although the basis states are the same, the irreducible spaces (i.e., also the orbital degeneracies) depend on the specific point group. They are shown in table 1.

$G^{\text{point}}$	$\Gamma^p$	$\{\varphi_b\}$
$[O_h, O, T_d, T_h]$	$[E_g, E, E, E_g]$ $[T_{2g}, T_2, T_2, T_g]$	$\varphi_u, \varphi_v$ $\varphi_\zeta, \varphi_\eta, \varphi_\xi$
$D_{6h}$	$A_{1g}$ $E_{2g}$ $E_{1g}$	$\varphi_u$ $\varphi_v, \varphi_\zeta$ $\varphi_\eta, \varphi_\xi$
$D_{4h}$	$A_{1g}$ $B_{1g}$ $B_{2g}$ $E_g$	$\varphi_u$ $\varphi_v$ $\varphi_\zeta$ $\varphi_\eta, \varphi_\xi$

**Table 1.** Irreducible representations  $\Gamma^p$  and corresponding basis states  $\varphi_b$  for  $d$ -orbitals in environments that belong to the crystallographic point groups  $O_h, O, T_d, T_h, D_{6h}, D_{4h}$ .

For the treatment of an  $f$ -shell we introduce two different sets of basis states, namely the ‘axial basis’

$$\begin{aligned} \varphi_a(r, \varphi, \theta) &= \frac{i}{\sqrt{2}} R_a(r) [Y_{3,-2}(\varphi, \theta) - Y_{3,2}(\varphi, \theta)] \\ &\sim xyz, \end{aligned} \quad (34)$$

$$\begin{aligned} \varphi_{x'}(r, \varphi, \theta) &= \frac{1}{\sqrt{2}} R_{x'}(r) [Y_{3,-1}(\varphi, \theta) - Y_{3,1}(\varphi, \theta)] \\ &\sim x(5z^2 - r^2), \end{aligned} \quad (35)$$

$$\begin{aligned} \varphi_{y'}(r, \varphi, \theta) &= \frac{i}{\sqrt{2}} R_{y'}(r) [Y_{3,-1}(\varphi, \theta) + Y_{3,1}(\varphi, \theta)] \\ &\sim y(5z^2 - r^2), \end{aligned} \quad (36)$$

$$\varphi_z(r, \varphi, \theta) = R_z(r) Y_{3,0}(\varphi, \theta) \sim z(5z^2 - 3r^2), \quad (37)$$

$$\begin{aligned} \varphi_{\alpha'}(r, \varphi, \theta) &= \frac{1}{\sqrt{2}} R_{\alpha'}(r) [Y_{3,-3}(\varphi, \theta) - Y_{3,3}(\varphi, \theta)] \\ &\sim x(x^2 - 3y^2), \end{aligned} \quad (38)$$

$$\begin{aligned} \varphi_{\beta'}(r, \varphi, \theta) &= \frac{i}{\sqrt{2}} R_{\beta'}(r) [Y_{3,-3}(\varphi, \theta) + Y_{3,3}(\varphi, \theta)] \\ &\sim y(3x^2 - y^2), \end{aligned} \quad (39)$$

$$\begin{aligned} \varphi_\gamma(r, \varphi, \theta) &= \frac{1}{\sqrt{2}} R_\gamma(r) [Y_{3,-2}(\varphi, \theta) + Y_{3,2}(\varphi, \theta)] \\ &\sim z(x^2 - y^2), \end{aligned} \quad (40)$$

and the ‘cubic basis’

$$\varphi_a(r, \varphi, \theta) \sim xyz, \quad (41)$$

$$\varphi_x(r, \varphi, \theta) \sim x(5x^2 - r^2), \quad (42)$$

$$\varphi_y(r, \varphi, \theta) \sim y(5y^2 - r^2), \quad (43)$$

$$\varphi_z(r, \varphi, \theta) \sim z(5z^2 - r^2), \quad (44)$$

$$\varphi_\alpha(r, \varphi, \theta) \sim x(y^2 - z^2), \quad (45)$$

$$\varphi_\beta(r, \varphi, \theta) \sim y(x^2 - z^2), \quad (46)$$

$$\varphi_\gamma(r, \varphi, \theta) \sim z(x^2 - y^2). \quad (47)$$

With these basis sets of states we can set up irreducible spaces for all our point groups. The results are summarised in table 2.

$G^{\text{point}}$	$\Gamma^p$	$\{\varphi_b\}$
$[O_h, O, T_d]$	$[A_{2u}, A_2, A_1]$	$\varphi_a$
	$[T_{1u}, T_1, T_2]$	$\varphi_x, \varphi_y, \varphi_z$
	$[T_{2u}, T_2, T_1]$	$\varphi_\alpha, \varphi_\beta, \varphi_\gamma$
$T_h$	$A_u$	$\varphi_a$
	$T_u$	$\varphi_x, \varphi_y, \varphi_z$
	$T_u$	$\varphi_\alpha, \varphi_\beta, \varphi_\gamma$
$D_{6h}$	$A_{2u}$	$\varphi_z$
	$B_{1u}$	$\varphi_{\alpha'}$
	$B_{2u}$	$\varphi_{\beta'}$
	$E_{1u}$	$\varphi_{x'}, \varphi_{y'}$
	$E_{2u}$	$\varphi_a, \varphi_\gamma$
$D_{4h}$	$A_{2u}$	$\varphi_z$
	$B_{1u}$	$\varphi_a$
	$B_{2u}$	$\varphi_\gamma$
	$E_u$	$\varphi_{x'}, \varphi_{y'}$
	$E_u$	$\varphi_{\alpha'}, \varphi_{\beta'}$

**Table 2.** Irreducible representations  $\Gamma^p$  and corresponding basis states  $\varphi_b$  for  $f$ -orbitals in environments that belong to the crystallographic point groups  $O_h, O, T_d, T_h, D_{6h}, D_{4h}$ .

#### 4. Coulomb matrix elements: full point group environment

First, we need to find the  $d$ -dimensional basis of joint eigenvectors  $\mathbf{c}^{(k)}$  of the matrices  $\tilde{\Gamma}(l)$  and  $\tilde{P}(i)$  and a basis  $\mathbf{d}^{(k')}$  of their orthogonal complement. This linear algebra problem is solved by standard algorithms provided by LAPACK.

Second, we have to solve equations (13), (14). The vectors  $\mathbf{c}^{(k)}$  that are provided by our numerical algorithm are somewhat arbitrary because any rotation among these vectors is permitted. Hence, the independent parameters  $I_k$  will usually be rather complicated linear combinations of Coulomb parameters  $U_{\mathbf{B}}$ . We therefore prefer to look for a set of  $d$  independent matrix elements  $U_{\mathbf{B}}^{(i)}$  (serving as parameters  $I_k$ ) and  $D-d$  dependent parameters  $U_{\mathbf{B}}^{(d)}$ . When we introduce the corresponding vectors  $\mathbf{U}^{(i),(d)}$  (and  $\mathbf{I}$  for  $I_k$ ), we can write the inversion of equations (13), (14) as

$$\begin{pmatrix} \mathbf{U}^{(i)} \\ \mathbf{U}^{(d)} \end{pmatrix} = \begin{pmatrix} \tilde{C}^{(i,i)} & \tilde{C}^{(i,d)} \\ \tilde{C}^{(d,i)} & \tilde{C}^{(d,d)} \end{pmatrix} \begin{pmatrix} \mathbf{I} \\ \mathbf{0} \end{pmatrix}, \quad (48)$$

where the matrix in (48) has the form

$$\begin{pmatrix} \tilde{C}^{(i,i)} & \tilde{C}^{(i,d)} \\ \tilde{C}^{(d,i)} & \tilde{C}^{(d,d)} \end{pmatrix} = \left( \mathbf{c}^{(1)}, \dots, \mathbf{c}^{(d)}, \mathbf{d}^{(1)}, \dots, \mathbf{d}^{(D-d)} \right).$$

Note that we can write equations (13), (14) in the form (48) because we are still free to choose the order of the indices in  $\mathbf{B}$ . We now demand that equation (48) has a unique solution for  $\mathbf{U}^{(d)}$  and  $\mathbf{I}$  as a function of  $\mathbf{U}^{(i)}$ . This is the case when the matrix  $\tilde{C}^{(i,i)}$  is regular, i.e.,

$$|\tilde{C}^{(i,i)}| \neq 0. \quad (49)$$

With this condition, we can systematically set up our list of independent parameters  $U_{\mathbf{B}}^{(i)}$  and determine the dependent parameters through

$$\mathbf{U}^{(d)} = \tilde{C}^{(d,i)} (\tilde{C}^{(i,i)})^{-1} \mathbf{U}^{(i)}. \quad (50)$$

With our formalism, we calculated the independent parameters  $U_{\mathbf{B}}^{(i)}$  and their relationship with all dependent parameters  $U_{\mathbf{B}}^{(d)}$  for a  $d$ -shell and an  $f$ -shell and for all the point groups introduced in section 3. As an example, we show the results for  $d$ -orbitals in a cubic environment in this section. The corresponding results for all other groups and/or  $f$ -orbitals are presented in Appendix B.

For a more convenient reading, we introduce the following notations for the Coulomb parameters

$$U(b) \equiv U_{b,b,b,b}, \quad (51)$$

$$U(b, b') \equiv U_{b,b',b',b}, \quad (52)$$

$$J(b, b') \equiv U_{b,b',b,b'}, \quad (53)$$

$$T(\bar{b}; b, b') \equiv U_{b,\bar{b},\bar{b},b'}, \quad (54)$$

$$A(\bar{b}; b, b') \equiv U_{b,\bar{b},b',\bar{b}}, \quad (55)$$

$$S(b_1, b_2; b_3, b_4) \equiv U_{b_1,b_2;b_3,b_4}, \quad (56)$$

which we use throughout this work. It is implicitly understood that all indices are mutually different in multi-orbital Coulomb parameters as, e.g. in eq. (56).

Equation (48) still leaves a lot of freedom in our choice of the independent parameters. We prefer to have as many independent parameters as possible that have an intuitive physical meaning. Hence we prioritise them along the order set by equations (51)-(56). This means that we first try to maximise the number of independent parameters of the form  $U(b)$ , then of the form  $U(b, b')$ , and so forth. In the remaining ambiguity with respect to the orbitals we prioritise orbitals along the order in equations (29)-(33), (34)-(47). For example, if we had to choose between  $U(v)$  and  $U(u)$  we would work with  $U(v)$  as an independent parameter.

For the five  $d$ -orbitals in a cubic environment, i.e., for the point groups  $O_h, O$ , and  $T_d$ , we find  $d = 10$  independent parameters, in agreement with reference [4]. These can, for example, be chosen as

$$U(v), U(\zeta), U(v, u), U(v, \zeta), U(u, \zeta), \\ U(\zeta, \eta), J(v, \zeta), J(v, \eta), J(\zeta, \eta), S(v, \zeta; \xi, \eta). \quad (57)$$

The dependent parameters are

$$U(u) = U(v) , \quad (58)$$

$$U(\eta) = U(\zeta) , \quad (59)$$

$$U(\xi) = U(\zeta) , \quad (60)$$

$$U(v, \eta) = \frac{1}{4}U(v, \zeta) + \frac{3}{4}U(u, \zeta) , \quad (61)$$

$$U(v, \xi) = \frac{1}{4}U(v, \zeta) + \frac{3}{4}U(u, \zeta) , \quad (62)$$

$$U(u, \eta) = \frac{3}{4}U(v, \zeta) + \frac{1}{4}U(u, \zeta) , \quad (63)$$

$$U(u, \xi) = \frac{3}{4}U(v, \zeta) + \frac{1}{4}U(u, \zeta) , \quad (64)$$

$$U(\zeta, \xi) = U(\zeta, \eta) , \quad (65)$$

$$U(\eta, \xi) = U(\zeta, \eta) , \quad (66)$$

$$J(v, u) = \frac{1}{2}U(v) - \frac{1}{2}U(v, u) , \quad (67)$$

$$J(u, \zeta) = -\frac{1}{3}J(v, \zeta) + \frac{4}{3}J(v, \eta) , \quad (68)$$

$$J(v, \xi) = J(v, \eta) , \quad (69)$$

$$J(u, \eta) = \frac{2}{3}J(v, \zeta) + \frac{1}{3}J(v, \eta) , \quad (70)$$

$$J(u, \xi) = \frac{2}{3}J(v, \zeta) + \frac{1}{3}J(v, \eta) , \quad (71)$$

$$J(\zeta, \xi) = J(\zeta, \eta) , \quad (72)$$

$$J(\eta, \xi) = J(\zeta, \eta) , \quad (73)$$

$$T(\eta; v, u) = -\frac{\sqrt{3}}{4}U(v, \zeta) + \frac{\sqrt{3}}{4}U(u, \zeta) , \quad (74)$$

$$T(\xi; v, u) = \frac{\sqrt{3}}{4}U(v, \zeta) - \frac{\sqrt{3}}{4}U(u, \zeta) , \quad (75)$$

$$A(\eta; v, u) = -\frac{1}{\sqrt{3}}J(v, \zeta) + \frac{1}{\sqrt{3}}J(v, \eta) , \quad (76)$$

$$A(\xi; v, u) = \frac{1}{\sqrt{3}}J(v, \zeta) - \frac{1}{\sqrt{3}}J(v, \eta) , \quad (77)$$

$$S(v, \zeta; \eta, \xi) = -S(v, \zeta; \xi, \eta) , \quad (78)$$

$$S(u, \zeta; \eta, \xi) = \frac{1}{\sqrt{3}}S(v, \zeta; \xi, \eta) , \quad (79)$$

$$S(u, \zeta; \xi, \eta) = \frac{1}{\sqrt{3}}S(v, \zeta; \xi, \eta) , \quad (80)$$

$$S(u, \eta; \xi, \zeta) = -\frac{2}{\sqrt{3}}S(v, \zeta; \xi, \eta) . \quad (81)$$

In this list, as in all corresponding lists in this work, we specify only one of the (up to eight) Coulomb parameters that differ just by a permutation of the form (26). Moreover, all parameters that are not listed vanish due to symmetry.

Note that the coefficients in all lists of dependent parameters come out of our numerical algorithm in digital form. We wrote a separate code that reliably identifies the analytical form of these digits, e.g., 0.5773502691896258 is identified as  $1/\sqrt{3}$ . This program also generates the L<sup>A</sup>T<sub>E</sub>X code of all formulae. Therefore, we are confident that they are free of

misprints.

## 5. Spherical approximation

The number of independent parameters determined in section 4 and Appendix B varies between 10 ( $d$ -orbitals in a  $O_h$  environment) and 65 ( $f$ -orbitals in a  $D_{4h}$  environment). When a full  $d$ -shell or  $f$ -shell was considered such numbers are too large if we aimed to determine them from meaningful fits to experiments. The localised nature of these orbitals, however, allows us to formulate sensible approximations that reduce the number of independent parameters significantly. The simplest one is the ‘spherical approximation’ which makes two assumptions.

- (i) The radial wave functions in equations (29)-(33) and in equations (34)-(47) are assumed to be orbital-independent. This means that the  $n_o = 5$   $d$ -orbitals or  $n_o = 7$   $f$ -orbitals form a representation space of the total angular momentum with  $j = 2$  and  $j = 3$ , respectively.
- ii) The two-particle interaction in (6) is assumed to be invariant under all orthogonal transformations, i.e.,

$$f(\mathbf{r}, \mathbf{r}') = f(|\mathbf{r} - \mathbf{r}'|). \quad (82)$$

As a generalisation of equations (10) and (11), these two assumptions lead to

$$\mathbf{U} = \tilde{\Gamma}(\tilde{D}) \cdot \mathbf{U} , \quad (83)$$

$$\Gamma_{\mathbf{B}, \mathbf{B}}(\tilde{D}) = \Gamma_{\tilde{b}_1, b_1}(\tilde{D}) \dots \Gamma_{\tilde{b}_4, b_4}(\tilde{D}) . \quad (84)$$

where  $\tilde{D}$  can be any real, orthogonal matrix. When the matrices  $\tilde{D}$  are chosen randomly, already two of this infinite number of equations contain all the information, and remain to be evaluated. Combined with the permutation equations (28), we can use the method of section 4 to determine a set of independent Coulomb integrals as well as their relationship with the dependent parameters.

For five  $d$ -orbitals, we obtain three independent parameters, which we may chose as

$$U(v), U(v, u), U(v, \zeta) . \quad (85)$$

The dependent parameters are then given by

$$U(u) = U(v) , \quad (86)$$

$$U(\zeta) = U(v) , \quad (87)$$

$$U(\eta) = U(v) , \quad (88)$$

$$U(u, \zeta) = U(v, u) , \quad (89)$$

$$U(v, \eta) = \frac{3}{4}U(v, u) + \frac{1}{4}U(v, \zeta) , \quad (90)$$

$$U(v, \xi) = \frac{3}{4}U(v, u) + \frac{1}{4}U(v, \zeta) , \quad (91)$$

$$U(u, \eta) = \frac{1}{4}U(v, u) + \frac{3}{4}U(v, \zeta) , \quad (92)$$

$$U(\zeta, \eta) = \frac{3}{4}U(v, u) + \frac{1}{4}U(v, \zeta), \quad (93)$$

$$U(\eta, \xi) = \frac{3}{4}U(v, u) + \frac{1}{4}U(v, \zeta), \quad (94)$$

$$J(v, u) = \frac{1}{2}U(v) - \frac{1}{2}U(v, u), \quad (95)$$

$$J(v, \zeta) = \frac{1}{2}U(v) - \frac{1}{2}U(v, \zeta), \quad (96)$$

$$J(v, \eta) = \frac{1}{2}U(v) - \frac{3}{8}U(v, u) - \frac{1}{8}U(v, \zeta), \quad (97)$$

$$J(u, \zeta) = \frac{1}{2}U(v) - \frac{1}{2}U(v, u), \quad (98)$$

$$J(v, \xi) = \frac{1}{2}U(v) - \frac{3}{8}U(v, u) - \frac{1}{8}U(v, \zeta), \quad (99)$$

$$J(u, \eta) = \frac{1}{2}U(v) - \frac{1}{8}U(v, u) - \frac{3}{8}U(v, \zeta), \quad (100)$$

$$J(\zeta, \eta) = \frac{1}{2}U(v) - \frac{3}{8}U(v, u) - \frac{1}{8}U(v, \zeta), \quad (101)$$

$$J(\eta, \xi) = \frac{1}{2}U(v) - \frac{3}{8}U(v, u) - \frac{1}{8}U(v, \zeta), \quad (102)$$

$$T(\eta; v, u) = \frac{\sqrt{3}}{4}U(v, u) - \frac{\sqrt{3}}{4}U(v, \zeta), \quad (103)$$

$$A(\eta; v, u) = -\frac{\sqrt{3}}{8}U(v, u) + \frac{\sqrt{3}}{8}U(v, \zeta), \quad (104)$$

$$S(v, \zeta; \xi, \eta) = -\frac{3}{8}U(v, u) + \frac{3}{8}U(v, \zeta), \quad (105)$$

$$S(v, \zeta; \eta, \xi) = \frac{3}{8}U(v, u) - \frac{3}{8}U(v, \zeta), \quad (106)$$

$$S(u, \eta; \xi, \zeta) = \frac{\sqrt{3}}{4}U(v, u) - \frac{\sqrt{3}}{4}U(v, \zeta), \quad (107)$$

$$S(u, \zeta; \eta, \xi) = -\frac{\sqrt{3}}{8}U(v, u) + \frac{\sqrt{3}}{8}U(v, \zeta). \quad (108)$$

This list only contains all *finite* dependent parameters that we specified in section 4 and Appendix B. All other Coulomb parameters can be calculated as a function of (85) using the results given in these two sections. For convenience, we provide a list for all (non-zero) Coulomb parameters in the supplementary material.

The corresponding results for *f*-orbitals are given in Appendix C.

## 6. First order corrections to the spherical approximation

In cases where the spherical approximation is not accurate enough, it is desirable to have a method that systemically improves it. For its derivation, we assume that the radial wave functions in (29)-(33) and (34)-(47) differ only slight from each other, i.e.,

$$R_b(r) \approx R(r) + \delta R_b(r). \quad (109)$$

Then, we can linearise the Coulomb matrix elements with respect to the small perturbations  $\delta R_b(r)$ ,

$$U_{b_1, b_2, b_3, b_4} \approx U_{b_1, b_2, b_3, b_4}^{\text{SA}} + \delta U_{b_1, b_2, b_3, b_4}, \quad (110)$$

where  $U_{b_1, b_2, b_3, b_4}^{\text{SA}}$  is the corresponding result from the spherical approximation and

$$\delta U_{b_1, b_2, b_3, b_4} \equiv \bar{U}_{b'_1, b_2, b_3, b_4} + \bar{U}_{b_1, b'_2, b_3, b_4} + \bar{U}_{b_1, b_2, b'_3, b_4} + \bar{U}_{b_1, b_2, b_3, b'_4}. \quad (111)$$

The matrix elements  $\bar{U}...$  are defined as in (6) with orbitals  $\varphi_{b_i}$  and  $\varphi_{b'_i}$  that have radial wave function  $R(r)$  and  $\delta R_{b_i}(r)$ , respectively.

Our first aim is now to identify independent and dependent parameters  $\bar{U}...$  and their relationships. To this end, we enlarge our orbital basis (from  $n_o$  to  $n'_o$ ) by introducing some auxiliary wave functions. These form a  $j = 2$  or  $j = 3$  representation spaces for each set of states  $\varphi_{b'_i}$  that belong to the same representation of the point group. For example, in the case of *d*-orbitals in a cubic environment, we end up with  $n'_o = 3n_o = 15$  orbital wave functions. These are

- (i) Five *d*-orbitals with a radial wave function  $R(r)$ .
- (ii) Five *d*-orbitals with the same radial wave function  $\delta R_u(r) = \delta R_v(r)$ , including three auxiliary  $t_{2g}$  orbitals.
- (iii) Five *d*-orbitals with the same radial wave function  $\delta R_\zeta(r) = \delta R_\eta(r) = \delta R_\xi(r)$ , including two auxiliary  $e_g$  orbitals.

We introduce the familiar multiple indices  $\bar{\mathbf{B}}$  as in eq. (9), however, with the indices  $b_i$  ranging from unity to  $n'_o$ . Each of the  $n'_o/n_o$  orbital subspaces transforms like a  $j = 2$  or  $j = 3$  representation. Hence, we obtain the equation (83) as in the spherical approximation but now for the parameters  $\bar{U}_{\bar{\mathbf{B}}}$ . Together with the corresponding equation of the form (28) we can determine independent and dependent parameters  $\bar{U}_{\bar{\mathbf{B}}}^{(i)}$  and  $\bar{U}_{\bar{\mathbf{B}}}^{(d)}$  with the same method as in section 4.

In principle, the problem is solved with this approach because, with the parameters  $\bar{U}_{\bar{\mathbf{B}}}^{(i, d)}$  at hand, we are able to calculate the variations (111) as a function of  $\bar{U}_{\bar{\mathbf{B}}}^{(i)}$ ,

$$\delta U_{\mathbf{B}} = \delta U_{\mathbf{B}}(\{\bar{U}_{\bar{\mathbf{B}}}^{(i)}\}). \quad (112)$$

However, this formulation leaves room for improvement for two reasons.

- (i) The naive selection of some independent parameters  $\bar{U}_{\bar{\mathbf{B}}}^{(i)}$  will also lead to variations of parameters  $U_{\mathbf{B}}$  which have already been chosen as independent parameters in the spherical approximation, see equations (85) and (C.1). Therefore, the spherical approximation and its first order corrections would be mixed up and could not be easily distinguished.
- (ii) The parameters  $\bar{U}_{\bar{\mathbf{B}}}^{(i)}$  have no intuitive physical meaning because only in their sum (111) they define the variation of a Coulomb matrix element.

Both problems can be readily addressed when we use the linear equations (112) to express the  $d'$  independent parameters  $\bar{U}_{\mathbf{B}}^{(i)}$  by some set of  $d'$  independent variations  $\delta U_{\mathbf{B}}^{(i)}$ . The latter set should contain the independent parameters from the spherical approximation so that we overcome the problem (i).

As an example, we consider the familiar case of  $d$ -orbitals in a cubic environment. Here, we obtain as independent variations  $\delta U_{\mathbf{B}}^{(i)}$ ,

$$\begin{aligned} \delta U(v), \delta U(v, u), \delta U(v, \zeta), \\ \delta U(\zeta), \delta U(u, \zeta), \delta U(\zeta, \eta) . \end{aligned} \quad (113)$$

The first line contains the independent parameters from the spherical approximation. Since their relation to all other parameters is already fully covered in equations (58)-(81), we only need to document the first-order changes introduced by the parameters in (113). In cubic symmetry these are

$$\delta J(v, \zeta) = \frac{1}{4} \delta U(\zeta) , \quad (114)$$

$$\delta J(v, \eta) = \frac{1}{4} \delta U(\zeta) - \frac{3}{8} \delta U(u, \zeta) , \quad (115)$$

$$\delta J(\zeta, \eta) = \frac{1}{2} \delta U(\zeta) - \frac{1}{2} \delta U(\zeta, \eta) , \quad (116)$$

$$\delta S(v, \zeta; \xi, \eta) = -\frac{27}{16} \delta U(u, \zeta) + \frac{3}{4} \delta U(\zeta, \eta) . \quad (117)$$

Note that, unlike the spherical approximation, the first-order correction depends on the point group that is considered. We present the results for all other point groups and/or  $f$ -orbitals in Appendix D. There we drop the variations of the parameters (85) and (C.1) because they are already covered by the corresponding formulae in section 5 and Appendix C.

Again, we provide the results for the independent parameters only that we specified in section 4 and Appendix B. All other Coulomb parameter variations can be calculated using the results given in these two sections. For convenience we provide a full list of all (non-zero) Coulomb parameter variations in the supplementary material.

## 7. Summary

In this work, we presented a comprehensive study of symmetries among Coulomb matrix elements of  $d$ -orbitals and  $f$ -orbitals in crystallographic point group environments. Such matrix elements are needed in all theoretical investigations that are based on Hubbard-type multi-orbital models. For all considered point groups ( $O_h$ ,  $O$ ,  $T_d$ ,  $T_h$ ,  $D_{6h}$ , and  $D_{4h}$ ) we determined an irreducible sub-set of independent Coulomb matrix elements and their relationship with all other matrix elements. Besides this evaluation of the full point-group problem, we also present results for the spherical approximation and a first-order correction to it.

Although our results are rather general in their inclusion of all orbitals of the  $d$ -shell and  $f$ -shell, they can be readily applied to situations where only a subset of orbitals needs to be taken into account in a theoretical study on a specific material.

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## Appendix A. Number of independent Coulomb interaction parameters

The number  $d$  of independent Coulomb interaction parameters is one of the results which one obtains from the explicit solution of equations (10), (28). Here we explain how  $d$  can be determined without that solution.

In equation (27) we introduced the eight ( $D$ -dimensional) representation matrices  $\hat{P}(i)$  of  $G^{\text{perm}}$ . Note that these matrices are real and symmetric because we have  $\hat{P}_i^{-1} = \hat{P}_i$  for all our permutations.

The permutation group dissects the basis states  $|\mathbf{B}\rangle$  into disjoint sets  $S^{(z)}$  of states that are connected by at least one permutation, i.e.,

$$|\mathbf{B}\rangle, |\mathbf{B}'\rangle \in S^{(z)} \Leftrightarrow \exists \hat{P}_i \text{ with } \langle \mathbf{B} | \hat{P}_i | \mathbf{B}' \rangle \neq 0 . \quad (\text{A.1})$$

The number of elements in  $S^{(z)}$  is denoted as  $N_z$  ( $= 1, \dots, 8$ ). For example,

$$N_z = 1 : S^{(z)} = \{(b_1, b_1, b_1, b_1)\} ; \quad (\text{A.2})$$

$$N_z = 4 : S^{(z)} = \{(b_1, b_2, b_2, b_2), (b_2, b_1, b_2, b_2), \\ (b_2, b_2, b_1, b_2), (b_2, b_2, b_2, b_1)\} ; \quad (\text{A.3})$$

$$N_z = 4 : S^{(z)} = \{(b_1, b_1, b_2, b_2), (b_1, b_2, b_1, b_2), \\ (b_2, b_1, b_2, b_1), (b_2, b_2, b_1, b_1)\} . \quad (\text{A.4})$$

With a representative  $|\mathbf{B}^{(z)}\rangle$  of each set  $S^{(z)}$ , we define the states

$$|\bar{\mathbf{B}}^{(z)}\rangle \equiv \frac{\sqrt{N_z}}{8} \sum_i \hat{P}_i |\mathbf{B}^{(z)}\rangle \quad (\text{A.5})$$

$$= \frac{\sqrt{N_z}}{8} \sum_i \sum_{\mathbf{B}} P_{\mathbf{B}, \mathbf{B}^{(z)}}(i) |\mathbf{B}\rangle \quad (\text{A.6})$$

that form an orthogonal and normalised basis for the ( $d_p$ -dimensional) space of all states that obey equations (28). With this basis we may define the following  $d_p$ -dimensional representation of  $G^{\text{point}}$ ,

$$\Gamma_{z,z'}(l) \equiv \langle \bar{\mathbf{B}}^{(z)} | \hat{T}_l | \bar{\mathbf{B}}^{(z')} \rangle . \quad (\text{A.7})$$

Using equation (20) we then obtain

$$d = \frac{1}{g} \sum_l \sum_z \Gamma_{z,z}(l) . \quad (\text{A.8})$$



This equation can be further evaluated,

$$d = \frac{1}{g} \sum_{z,l} \langle \bar{\mathbf{B}}^{(z)} | \hat{T}_l | \bar{\mathbf{B}}^{(z)} \rangle \quad (\text{A.9})$$

$$= \frac{1}{64g} \sum_{z,l} N_z \sum_{i,j} \sum_{\mathbf{B},\mathbf{B}'} P_{\mathbf{B},\mathbf{B}^{(z)}}(i) P_{\mathbf{B}',\mathbf{B}^{(z)}}(j) \Gamma_{\mathbf{B},\mathbf{B}'}(l) .$$

Now we use the fact that, by choosing a different representative  $|\mathbf{B}^{(z)}\rangle$ , the state  $|\bar{\mathbf{B}}^{(z)}\rangle$  remains unchanged. Hence, we find that

$$\sum_z N_z \sum_{i,j} \sum_{\mathbf{B},\mathbf{B}'} P_{\mathbf{B},\mathbf{B}^{(z)}}(i) P_{\mathbf{B}',\mathbf{B}^{(z)}}(j) \quad (\text{A.10})$$

$$= \sum_z \frac{N_z}{N_z} \sum_{\mathbf{B}'' \in S^{(z)}} \sum_{i,j} \sum_{\mathbf{B},\mathbf{B}'} P_{\mathbf{B},\mathbf{B}''}(i) P_{\mathbf{B}',\mathbf{B}''}(j) . \quad (\text{A.11})$$

Since

$$\sum_z \sum_{\mathbf{B}'' \in S^{(z)}} = \sum_{\mathbf{B}''} \quad (\text{A.12})$$

we finally obtain

$$d = \frac{1}{64g} \sum_l \sum_{i,j} \sum_{\mathbf{B},\mathbf{B}'} P_{\mathbf{B},\mathbf{B}'}(i \circ j) \Gamma_{\mathbf{B},\mathbf{B}'}(l) \quad (\text{A.13})$$

$$= \frac{1}{8g} \sum_l \sum_i \sum_{\mathbf{B},\mathbf{B}'} P_{\mathbf{B},\mathbf{B}'}(i) \Gamma_{\mathbf{B},\mathbf{B}'}(l) \quad (\text{A.14})$$

$$= \frac{1}{8g} \sum_{l,i} \sum_{\mathbf{B}} [\tilde{P}(i) \cdot \tilde{\Gamma}(l)]_{\mathbf{B},\mathbf{B}} . \quad (\text{A.15})$$

This equation is obviously a generalisation of (21) in the presence of the additional permutation symmetry.

## Appendix B. Coulomb matrix elements: full point group environment

### Appendix B.1. d-orbitals, group $T_h$

Independent parameters:

$$U(v), U(\zeta), U(v, u), U(v, \zeta), U(u, \zeta), \quad (\text{B.1})$$

$$U(v, \eta), U(\zeta, \eta), J(v, \zeta), J(v, \eta), J(u, \zeta),$$

$$J(\zeta, \eta), S(v, \zeta; \xi, \eta), S(v, \eta; \xi, \zeta),$$

Dependent parameters:

$$U(u) = U(v) , \quad (\text{B.2})$$

$$U(\eta) = U(\zeta) ,$$

$$U(\xi) = U(\zeta) ,$$

$$U(v, \xi) = \frac{1}{2}U(v, \zeta) + \frac{3}{2}U(u, \zeta) - U(v, \eta) ,$$

$$U(u, \eta) = U(v, \zeta) + U(u, \zeta) - U(v, \eta) ,$$

$$U(u, \xi) = \frac{1}{2}U(v, \zeta) - \frac{1}{2}U(u, \zeta) + U(v, \eta) ,$$

$$U(\zeta, \xi) = U(\zeta, \eta) ,$$

$$U(\eta, \xi) = U(\zeta, \eta) ,$$

$$J(v, u) = \frac{1}{2}U(v) - \frac{1}{2}U(v, u) ,$$

$$J(v, \xi) = \frac{1}{2}J(v, \zeta) - J(v, \eta) + \frac{3}{2}J(u, \zeta) ,$$

$$J(u, \eta) = J(v, \zeta) - J(v, \eta) + J(u, \zeta) ,$$

$$J(u, \xi) = \frac{1}{2}J(v, \zeta) + J(v, \eta) - \frac{1}{2}J(u, \zeta) ,$$

$$J(\zeta, \xi) = J(\zeta, \eta) ,$$

$$J(\eta, \xi) = J(\zeta, \eta) ,$$

$$T(\zeta; v, u) = -\frac{1}{\sqrt{12}}U(v, \zeta) - \frac{\sqrt{3}}{2}U(u, \zeta) + \frac{2}{\sqrt{3}}U(v, \eta) ,$$

$$T(\eta; v, u) = -\frac{1}{\sqrt{12}}U(v, \zeta) + \frac{\sqrt{3}}{2}U(u, \zeta) - \frac{1}{\sqrt{3}}U(v, \eta) ,$$

$$T(\xi; v, u) = \frac{1}{\sqrt{3}}U(v, \zeta) - \frac{1}{\sqrt{3}}U(v, \eta) ,$$

$$A(\zeta; v, u) = -\frac{1}{\sqrt{12}}J(v, \zeta) + \frac{2}{\sqrt{3}}J(v, \eta) - \frac{\sqrt{3}}{2}J(u, \zeta) ,$$

$$A(\eta; v, u) = -\frac{1}{\sqrt{12}}J(v, \zeta) - \frac{1}{\sqrt{3}}J(v, \eta) + \frac{\sqrt{3}}{2}J(u, \zeta) ,$$

$$A(\xi; v, u) = \frac{1}{\sqrt{3}}J(v, \zeta) - \frac{1}{\sqrt{3}}J(v, \eta) ,$$

$$S(v, \zeta; \eta, \xi) = -S(v, \zeta; \xi, \eta) - S(v, \eta; \xi, \zeta) ,$$

$$S(u, \zeta; \eta, \xi) = \frac{1}{\sqrt{3}}S(v, \zeta; \xi, \eta) - \frac{1}{\sqrt{3}}S(v, \eta; \xi, \zeta) ,$$

$$S(u, \zeta; \xi, \eta) = \frac{1}{\sqrt{3}}S(v, \zeta; \xi, \eta) + \frac{2}{\sqrt{3}}S(v, \eta; \xi, \zeta) ,$$

$$S(u, \eta; \xi, \zeta) = -\frac{2}{\sqrt{3}}S(v, \zeta; \xi, \eta) - \frac{1}{\sqrt{3}}S(v, \eta; \xi, \zeta) .$$

### Appendix B.2. d-orbitals, group $D_{6h}$

Independent parameters:

$$U(v), U(u), U(\eta), U(v, u), U(v, \zeta), \quad (\text{B.3})$$

$$U(v, \eta), U(v, \xi), U(u, \eta), U(\eta, \xi), J(v, u),$$

$$J(v, \eta), J(v, \xi), J(u, \eta), T(\zeta; v, u), T(\eta; v, u),$$

$$A(\eta; v, u), S(v, \zeta; \eta, \xi) .$$

Dependent parameters:

$$U(\zeta) = U(v) , \quad (\text{B.4})$$

$$U(\xi) = U(\eta) ,$$

$$U(u, \zeta) = U(v, u) ,$$

$$U(u, \xi) = U(u, \eta) ,$$

$$U(\zeta, \eta) = U(v, \xi) ,$$

$$U(\zeta, \xi) = U(v, \eta) ,$$

$$J(v, \zeta) = \frac{1}{2}U(v) - \frac{1}{2}U(v, \zeta) ,$$

$$J(u, \zeta) = J(v, u) ,$$

$$J(u, \xi) = J(u, \eta) ,$$

$$J(\zeta, \eta) = J(v, \xi) ,$$

$$J(\zeta, \xi) = J(v, \eta) ,$$

$$J(\eta, \xi) = \frac{1}{2}U(\eta) - \frac{1}{2}U(\eta, \xi) ,$$

$$\begin{aligned}
T(\xi; v, u) &= -T(\eta; v, u) , \\
A(v; v, u) &= -T(\zeta; v, u) , \\
A(\zeta; v, u) &= T(\zeta; v, u) , \\
A(\xi; v, u) &= -A(\eta; v, u) , \\
S(v, \zeta; \xi, \eta) &= -J(v, \eta) + J(v, \xi) - S(v, \zeta; \eta, \xi) , \\
S(v, \eta; \xi, \zeta) &= -\frac{1}{2}U(v, \eta) + \frac{1}{2}U(v, \xi) , \\
S(u, \zeta; \eta, \xi) &= A(\eta; v, u) , \\
S(u, \zeta; \xi, \eta) &= A(\eta; v, u) , \\
S(u, \eta; \xi, \zeta) &= T(\eta; v, u) .
\end{aligned}$$

### Appendix B.3. d-orbitals, group $D_{4h}$

Independent parameters:

$$\begin{aligned}
U(v), U(u), U(\zeta), U(\eta), U(v, u), \\
U(v, \zeta), U(u, \zeta), U(v, \eta), U(u, \eta), U(\zeta, \eta), \\
U(\eta, \xi), J(v, u), J(v, \zeta), J(v, \eta), J(u, \zeta), \\
J(u, \eta), J(\zeta, \eta), J(\eta, \xi), T(\eta; v, u), A(\eta; v, u), \\
S(v, \zeta; \xi, \eta), S(u, \zeta; \eta, \xi), S(u, \eta; \xi, \zeta) .
\end{aligned} \tag{B.5}$$

Dependent parameters:

$$\begin{aligned}
U(\xi) &= U(\eta) , \\
U(v, \xi) &= U(v, \eta) , \\
U(u, \xi) &= U(u, \eta) , \\
U(\zeta, \xi) &= U(\zeta, \eta) , \\
J(v, \xi) &= J(v, \eta) , \\
J(u, \xi) &= J(u, \eta) , \\
J(\zeta, \xi) &= J(\zeta, \eta) , \\
T(\xi; v, u) &= -T(\eta; v, u) , \\
A(\xi; v, u) &= -A(\eta; v, u) , \\
S(v, \zeta; \eta, \xi) &= -S(v, \zeta; \xi, \eta) , \\
S(u, \zeta; \xi, \eta) &= S(u, \zeta; \eta, \xi) .
\end{aligned} \tag{B.6}$$

### Appendix B.4. f-orbitals, groups $O_h$ , $O$ , $T_d$

Independent parameters:

$$\begin{aligned}
U(a), U(x), U(\alpha), U(a, x), U(x, y), \\
U(a, \alpha), U(x, \alpha), U(x, \beta), U(\alpha, \beta), J(a, x), \\
J(x, y), J(a, \alpha), J(x, \alpha), J(y, \alpha), J(\alpha, \beta), \\
T(y; x, \alpha), T(\beta; x, \alpha), A(x; x, \beta), A(\beta; x, \alpha), \\
S(a, x; z, y), S(a, x; \beta, z), S(a, x; \gamma, \beta), S(a, \alpha; \beta, z), \\
S(x, \alpha; \beta, y), S(x, y; \alpha, \beta), S(x, y; \beta, \alpha) .
\end{aligned} \tag{B.7}$$

Dependent parameters:

$$\begin{aligned}
U(y) &= U(x) , \\
U(z) &= U(x) , \\
U(\beta) &= U(\alpha) , \\
U(\gamma) &= U(\alpha) , \\
U(a, y) &= U(a, x) ,
\end{aligned} \tag{B.8}$$

$$\begin{aligned}
U(a, z) &= U(a, x) , \\
U(x, z) &= U(x, y) , \\
U(a, \beta) &= U(a, \alpha) , \\
U(y, z) &= U(x, y) , \\
U(a, \gamma) &= U(a, \alpha) , \\
U(y, \alpha) &= U(x, \beta) , \\
U(z, \alpha) &= U(x, \beta) , \\
U(x, \gamma) &= U(x, \beta) , \\
U(y, \beta) &= U(x, \alpha) , \\
U(z, \beta) &= U(x, \beta) , \\
U(y, \gamma) &= U(x, \beta) , \\
U(z, \gamma) &= U(x, \alpha) , \\
U(\alpha, \gamma) &= U(\alpha, \beta) , \\
U(\beta, \gamma) &= U(\alpha, \beta) , \\
J(a, y) &= J(a, x) , \\
J(a, z) &= J(a, x) , \\
J(x, z) &= J(x, y) , \\
J(a, \beta) &= J(a, \alpha) , \\
J(y, z) &= J(x, y) , \\
J(x, \beta) &= J(y, \alpha) , \\
J(a, \gamma) &= J(a, \alpha) , \\
J(y, \beta) &= J(x, \alpha) , \\
J(x, \gamma) &= J(y, \alpha) , \\
J(z, \alpha) &= J(y, \alpha) , \\
J(z, \beta) &= J(y, \alpha) , \\
J(y, \gamma) &= J(y, \alpha) , \\
J(z, \gamma) &= J(x, \alpha) , \\
J(\alpha, \gamma) &= J(\alpha, \beta) , \\
J(\beta, \gamma) &= J(\alpha, \beta) , \\
T(x; y, \beta) &= T(y; x, \alpha) , \\
T(x; z, \gamma) &= T(y; x, \alpha) , \\
T(z; x, \alpha) &= -T(y; x, \alpha) , \\
T(z; y, \beta) &= -T(y; x, \alpha) , \\
T(y; z, \gamma) &= -T(y; x, \alpha) , \\
T(\alpha; y, \beta) &= T(\beta; x, \alpha) , \\
T(\gamma; x, \alpha) &= -T(\beta; x, \alpha) , \\
T(\alpha; z, \gamma) &= T(\beta; x, \alpha) , \\
T(\beta; z, \gamma) &= -T(\beta; x, \alpha) , \\
T(\gamma; y, \beta) &= -T(\beta; x, \alpha) , \\
A(y; x, \alpha) &= A(x; x, \beta) , \\
A(x; x, \gamma) &= A(x; x, \beta) , \\
A(z; x, \alpha) &= -A(x; x, \beta) , \\
A(y; y, \gamma) &= -A(x; x, \beta) , \\
A(z; y, \beta) &= -A(x; x, \beta) ,
\end{aligned}$$

$$\begin{aligned}
A(\alpha; y, \beta) &= A(\beta; x, \alpha) , & U(a, z) &= U(a, x) , \\
A(\alpha; z, \gamma) &= A(\beta; x, \alpha) , & U(x, z) &= U(x, y) , \\
A(\gamma; x, \alpha) &= -A(\beta; x, \alpha) , & U(a, \beta) &= U(a, \alpha) , \\
A(\beta; z, \gamma) &= -A(\beta; x, \alpha) , & U(y, z) &= U(x, y) , \\
A(\gamma; y, \beta) &= -A(\beta; x, \alpha) , & U(a, \gamma) &= U(a, \alpha) , \\
S(a, y; z, x) &= S(a, x; z, y) , & U(z, \alpha) &= U(x, \beta) , \\
S(a, x; y, z) &= S(a, x; z, y) , & U(x, \gamma) &= U(y, \alpha) , \\
S(a, z; \alpha, y) &= -S(a, x; \beta, z) , & U(y, \beta) &= U(x, \alpha) , \\
S(a, z; \beta, x) &= -S(a, x; \beta, z) , & U(z, \beta) &= U(y, \alpha) , \\
S(a, x; \gamma, y) &= S(a, x; \beta, z) , & U(y, \gamma) &= U(x, \beta) , \\
S(a, y; \alpha, z) &= S(a, x; \beta, z) , & U(z, \gamma) &= U(x, \alpha) , \\
S(a, y; \gamma, x) &= -S(a, x; \beta, z) , & U(\alpha, \gamma) &= U(\alpha, \beta) , \\
S(a, z; \alpha, \beta) &= S(a, x; \gamma, \beta) , & U(\beta, \gamma) &= U(\alpha, \beta) , \\
S(a, \alpha; \gamma, y) &= -S(a, \alpha; \beta, z) , & J(a, y) &= J(a, x) , \\
S(a, y; \gamma, \alpha) &= -S(a, x; \gamma, \beta) , & J(a, z) &= J(a, x) , \\
S(a, z; \beta, \alpha) &= S(a, x; \gamma, \beta) , & J(x, z) &= J(x, y) , \\
S(a, x; \beta, \gamma) &= S(a, x; \gamma, \beta) , & J(a, \beta) &= J(a, \alpha) , \\
S(a, y; \alpha, \gamma) &= -S(a, x; \gamma, \beta) , & J(y, z) &= J(x, y) , \\
S(a, \beta; \gamma, x) &= S(a, \alpha; \beta, z) , & J(a, \gamma) &= J(a, \alpha) , \\
S(x, z; \alpha, \gamma) &= -S(x, y; \alpha, \beta) , & J(y, \beta) &= J(x, \alpha) , \\
S(x, z; \gamma, \alpha) &= -S(x, y; \beta, \alpha) , & J(x, \gamma) &= J(y, \alpha) , \\
S(x, \alpha; \gamma, z) &= -S(x, \alpha; \beta, y) , & J(z, \alpha) &= J(x, \beta) , \\
S(y, \beta; \gamma, z) &= S(x, \alpha; \beta, y) , & J(z, \beta) &= J(y, \alpha) , \\
S(y, z; \beta, \gamma) &= S(x, y; \alpha, \beta) , & J(y, \gamma) &= J(x, \beta) , \\
S(y, z; \gamma, \beta) &= S(x, y; \beta, \alpha) . & J(z, \gamma) &= J(x, \alpha) , \\
& & J(\alpha, \gamma) &= J(\alpha, \beta) , \\
& & J(\beta, \gamma) &= J(\alpha, \beta) , \\
& & T(a; y, \beta) &= T(a; x, \alpha) , \\
& & T(a; z, \gamma) &= T(a; x, \alpha) , \\
& & T(z; x, \alpha) &= T(x; y, \beta) , \\
& & T(x; z, \gamma) &= T(y; x, \alpha) , \\
& & T(z; y, \beta) &= T(y; x, \alpha) , \\
& & T(y; z, \gamma) &= T(x; y, \beta) , \\
& & T(\alpha; z, \gamma) &= T(\beta; x, \alpha) , \\
& & T(\gamma; x, \alpha) &= T(\alpha; y, \beta) , \\
& & T(\gamma; y, \beta) &= T(\beta; x, \alpha) , \\
& & T(\beta; z, \gamma) &= T(\alpha; y, \beta) , \\
& & A(a; a, \beta) &= A(a; a, \alpha) , \\
& & A(a; a, \gamma) &= A(a; a, \alpha) , \\
& & A(x; x, \gamma) &= A(y; x, \alpha) , \\
& & A(y; y, \beta) &= A(x; x, \alpha) , \\
& & A(z; x, \alpha) &= A(x; x, \beta) , \\
& & A(z; y, \beta) &= A(y; x, \alpha) , \\
& & A(y; y, \gamma) &= A(x; x, \beta) ,
\end{aligned}$$

#### Appendix B.5. *f*-orbitals, group $T_h$

Independent parameters:

$$\begin{aligned}
& U(a), U(x), U(\alpha), U(a, x), U(x, y), \\
& U(a, \alpha), U(x, \alpha), U(x, \beta), U(y, \alpha), U(\alpha, \beta), \\
& J(a, x), J(x, y), J(a, \alpha), J(x, \alpha), J(y, \alpha), \\
& J(x, \beta), J(\alpha, \beta), T(a; x, \alpha), T(y; x, \alpha), T(x; y, \beta), \\
& T(\alpha; y, \beta), T(\beta; x, \alpha), A(a; a, \alpha), A(x; x, \alpha), A(y; x, \alpha), \\
& A(x; x, \beta), A(\alpha; x, \alpha), A(\beta; x, \alpha), A(\alpha; y, \beta), \\
& S(a, x; z, y), S(a, y; \gamma, x), S(a, x; \gamma, y), S(a, x; z, \beta), \\
& S(x, y; \beta, \alpha), S(a, \alpha; \gamma, y), S(a, x; \gamma, \beta), S(a, y; \gamma, \alpha), \\
& S(x, \alpha; \beta, y), S(x, y; \alpha, \beta), S(a, \beta; \gamma, \alpha) .
\end{aligned} \tag{B.9}$$

Dependent parameters:

$$\begin{aligned}
& U(y) = U(x) , \\
& U(z) = U(x) , \\
& U(\beta) = U(\alpha) , \\
& U(\gamma) = U(\alpha) , \\
& U(a, y) = U(a, x) ,
\end{aligned} \tag{B.10}$$

$$\begin{aligned}
A(z; z, \gamma) &= A(x; x, \alpha) , \\
A(\alpha; z, \gamma) &= A(\beta; x, \alpha) , \\
A(\gamma; x, \alpha) &= A(\alpha; y, \beta) , \\
A(\beta; y, \beta) &= A(\alpha; x, \alpha) , \\
A(\beta; z, \gamma) &= A(\alpha; y, \beta) , \\
A(\gamma; y, \beta) &= A(\beta; x, \alpha) , \\
A(\gamma; z, \gamma) &= A(\alpha; x, \alpha) , \\
S(a, y; z, x) &= S(a, x; z, y) , \\
S(a, x; y, z) &= S(a, x; z, y) , \\
S(a, x; \beta, z) &= S(a, y; \gamma, x) , \\
S(a, y; z, \alpha) &= S(a, x; z, \beta) , \\
S(a, z; \alpha, y) &= S(a, y; \gamma, x) , \\
S(a, z; \beta, x) &= S(a, x; \gamma, y) , \\
S(a, y; \alpha, z) &= S(a, x; \gamma, y) , \\
S(a, x; y, \gamma) &= S(a, x; z, \beta) , \\
S(a, z; \alpha, \beta) &= S(a, y; \gamma, \alpha) , \\
S(a, y; \alpha, \gamma) &= S(a, x; \gamma, \beta) , \\
S(a, z; \beta, \alpha) &= S(a, x; \gamma, \beta) , \\
S(a, \beta; \gamma, x) &= S(a, \alpha; \gamma, y) , \\
S(a, x; \beta, \gamma) &= S(a, y; \gamma, \alpha) , \\
S(a, \alpha; \beta, z) &= S(a, \alpha; \gamma, y) , \\
S(x, \alpha; \gamma, z) &= S(x, \alpha; \beta, y) , \\
S(x, z; \gamma, \alpha) &= S(x, y; \beta, \alpha) , \\
S(x, z; \alpha, \gamma) &= S(x, y; \alpha, \beta) , \\
S(a, \alpha; \beta, \gamma) &= S(a, \beta; \gamma, \alpha) , \\
S(a, \alpha; \gamma, \beta) &= S(a, \beta; \gamma, \alpha) , \\
S(y, z; \gamma, \beta) &= S(x, y; \beta, \alpha) , \\
S(y, z; \beta, \gamma) &= S(x, y; \alpha, \beta) , \\
S(y, \beta; \gamma, z) &= S(x, \alpha; \beta, y) .
\end{aligned}$$

#### Appendix B.6. *f*-orbitals, group $D_{6h}$

Independent parameters:

$$\begin{aligned}
&U(a), U(x'), U(z), U(\alpha'), U(\beta'), \\
&U(a, x'), U(a, y'), U(a, z), U(x', y'), U(x', z), \\
&U(a, \alpha'), U(x', \alpha'), U(a, \beta'), U(a, \gamma), U(x', \beta'), \\
&U(z, \alpha'), U(z, \beta'), U(\alpha', \beta'), J(a, x'), J(a, y'), \\
&J(a, z), J(x', z), J(a, \alpha'), J(a, \beta'), J(x', \alpha'), \\
&J(x', \beta'), J(z, \alpha'), J(z, \beta'), J(\alpha', \beta'), T(a; x', \alpha'), \\
&T(a; y', \beta'), T(a; z, \gamma), T(y'; x', \alpha'), T(x'; y', \beta'), \\
&T(x'; z, \gamma), A(a; a, \alpha'), A(a; a, \beta'), A(x'; x', \gamma), \\
&S(a, x'; \gamma, y'), S(a, x'; z, \beta'), S(a, y'; z, \alpha'), \\
&S(a, z; \alpha', y'), S(a, z; \beta', x'), S(a, y'; \alpha', z), \\
&S(a, x'; \beta', z), S(x', y'; \beta', \alpha'), S(a, \alpha'; \gamma, \beta') .
\end{aligned} \tag{B.11}$$

Dependent parameters:

$$U(y') = U(x') , \tag{B.12}$$

$$\begin{aligned}
&U(\gamma) = U(a) , \\
&U(y', z) = U(x', z) , \\
&U(y', \alpha') = U(x', \alpha') , \\
&U(x', \gamma) = U(a, y') , \\
&U(y', \beta') = U(x', \beta') , \\
&U(y', \gamma) = U(a, x') , \\
&U(z, \gamma) = U(a, z) , \\
&U(\alpha', \gamma) = U(a, \alpha') , \\
&U(\beta', \gamma) = U(a, \beta') , \\
&J(x', y') = \frac{1}{2}U(x') - \frac{1}{2}U(x', y') , \\
&J(y', z) = J(x', z) , \\
&J(y', \alpha') = J(x', \alpha') , \\
&J(a, \gamma) = \frac{1}{2}U(a) - \frac{1}{2}U(a, \gamma) , \\
&J(y', \beta') = J(x', \beta') , \\
&J(x', \gamma) = J(a, y') , \\
&J(y', \gamma) = J(a, x') , \\
&J(z, \gamma) = J(a, z) , \\
&J(\alpha', \gamma) = J(a, \alpha') , \\
&J(\beta', \gamma) = J(a, \beta') , \\
&T(y'; z, \gamma) = -T(x'; z, \gamma) , \\
&T(\gamma; x', \alpha') = -T(a; x', \alpha') , \\
&T(\gamma; y', \beta') = -T(a; y', \beta') , \\
&A(x'; x', \alpha') = -T(y'; x', \alpha') , \\
&A(a; a, \gamma) = T(a; z, \gamma) , \\
&A(x'; x', \beta') = T(x'; y', \beta') , \\
&A(y'; x', \alpha') = T(y'; x', \alpha') , \\
&A(y'; y', \beta') = -T(x'; y', \beta') , \\
&A(y'; y', \gamma) = -A(x'; x', \gamma) , \\
&A(\gamma; x', \alpha') = -A(a; a, \alpha') , \\
&A(\gamma; y', \beta') = -A(a; a, \beta') , \\
&A(\gamma; z, \gamma) = -T(a; z, \gamma) , \\
&S(a, y'; z, x') = A(x'; x', \gamma) , \\
&S(a, x'; y', z) = T(x'; z, \gamma) , \\
&S(a, x'; z, y') = A(x'; x', \gamma) , \\
&S(a, x'; y', \gamma) = \frac{1}{2}U(a, x') - \frac{1}{2}U(a, y') , \\
&S(a, y'; \gamma, x') = J(a, x') - J(a, y') - S(a, x'; \gamma, y') , \\
&S(a, x'; \gamma, \beta') = A(a; a, \beta') , \\
&S(a, y'; \gamma, \alpha') = -A(a; a, \alpha') , \\
&S(a, \alpha'; \gamma, y') = -A(a; a, \alpha') , \\
&S(a, \beta'; \gamma, x') = A(a; a, \beta') , \\
&S(a, y'; \alpha', \gamma) = -T(a; x', \alpha') , \\
&S(a, x'; \beta', \gamma) = T(a; y', \beta') , \\
&S(x', y'; \alpha', \beta') = -S(x', y'; \beta', \alpha') ,
\end{aligned}$$

$$\begin{aligned}
S(x', z; \gamma, \alpha') &= -S(a, y'; \alpha', z), \\
S(x', z; \alpha', \gamma) &= -S(a, z; \alpha', y'), \\
S(x', \alpha'; \gamma, z) &= -S(a, y'; z, \alpha'), \\
S(a, \beta'; \gamma, \alpha') &= -S(a, \alpha'; \gamma, \beta'), \\
S(y', z; \gamma, \beta') &= S(a, x'; \beta', z), \\
S(y', z; \beta', \gamma) &= S(a, z; \beta', x'), \\
S(y', \beta'; \gamma, z) &= S(a, x'; z, \beta'),
\end{aligned}$$

#### Appendix B.7. $f$ -orbitals, group $D_{4h}$

Independent parameters:

$$\begin{aligned}
&U(a), U(x'), U(z), U(\alpha'), U(\gamma), \\
&U(a, x'), U(a, z), U(x', y'), U(x', z), U(a, \alpha'), \\
&U(x', \alpha'), U(a, \gamma), U(x', \beta'), U(z, \alpha'), U(x', \gamma), \\
&U(z, \gamma), U(\alpha', \beta'), U(\alpha', \gamma), J(a, x'), J(a, z), \\
&J(x', y'), J(x', z), J(a, \alpha'), J(x', \alpha'), J(y', \alpha'), \\
&J(a, \gamma), J(x', \gamma), J(z, \alpha'), J(\alpha', \beta'), J(z, \gamma), \\
&J(\alpha', \gamma), T(a; x', \alpha'), T(x'; y', \beta'), T(z; x', \alpha'), \\
&T(x'; z, \gamma), T(\alpha'; y', \beta'), T(\alpha'; z, \gamma), T(\gamma; x', \alpha'), \\
&A(a; a, \alpha'), A(x'; x', \alpha'), A(y'; x', \alpha'), A(z; x', \alpha'), \\
&A(x'; x', \gamma), A(\alpha'; x', \alpha'), A(\beta'; x', \alpha'), A(\gamma; x', \alpha'), \\
&A(\alpha'; z, \gamma), S(a, x'; z, y'), S(a, x'; y', z), S(a, x'; \gamma, y'), \\
&S(a, x'; z, \beta'), S(a, z; \alpha', y'), S(a, y'; \alpha', z), \\
&S(a, \beta'; \gamma, x'), S(x', \alpha'; \beta', y'), S(x', y'; \alpha', \beta'), \\
&S(a, z; \beta', \alpha'), S(x', y'; \beta', \alpha'), S(a, \alpha'; \beta', z), \\
&S(a, y'; \alpha', \gamma), S(a, x'; \gamma, \beta'), S(x', z; \alpha', \gamma), \\
&S(x', \alpha'; \gamma, z), S(x', z; \gamma, \alpha'), S(a, \alpha'; \gamma, \beta').
\end{aligned} \tag{B.13}$$

Dependent parameters:

$$\begin{aligned}
&U(y') = U(x'), \\
&U(\beta') = U(\alpha'), \\
&U(a, y') = U(a, x'), \\
&U(a, \beta') = U(a, \alpha'), \\
&U(y', z) = U(x', z), \\
&U(y', \alpha') = U(x', \beta'), \\
&U(y', \beta') = U(x', \alpha'), \\
&U(z, \beta') = U(z, \alpha'), \\
&U(y', \gamma) = U(x', \gamma), \\
&U(\beta', \gamma) = U(\alpha', \gamma), \\
&J(a, y') = J(a, x'), \\
&J(a, \beta') = J(a, \alpha'), \\
&J(y', z) = J(x', z), \\
&J(x', \beta') = J(y', \alpha'), \\
&J(y', \beta') = J(x', \alpha'), \\
&J(z, \beta') = J(z, \alpha'),
\end{aligned} \tag{B.14}$$

$$\begin{aligned}
J(y', \gamma) &= J(x', \gamma), \\
J(\beta', \gamma) &= J(\alpha', \gamma), \\
T(a; y', \beta') &= -T(a; x', \alpha'), \\
T(y'; x', \alpha') &= -T(x'; y', \beta'), \\
T(z; y', \beta') &= -T(z; x', \alpha'), \\
T(y'; z, \gamma) &= -T(x'; z, \gamma), \\
T(\beta'; x', \alpha') &= -T(\alpha'; y', \beta'), \\
T(\beta'; z, \gamma) &= -T(\alpha'; z, \gamma), \\
T(\gamma; y', \beta') &= -T(\gamma; x', \alpha'), \\
A(a; a, \beta') &= -A(a; a, \alpha'), \\
A(x'; x', \beta') &= -A(y'; x', \alpha'), \\
A(y'; y', \beta') &= -A(x'; x', \alpha'), \\
A(y'; y', \gamma) &= -A(x'; x', \gamma), \\
A(z; y', \beta') &= -A(z; x', \alpha'), \\
A(\alpha'; y', \beta') &= -A(\beta'; x', \alpha'), \\
A(\beta'; y', \beta') &= -A(\alpha'; x', \alpha'), \\
A(\beta'; z, \gamma) &= -A(\alpha'; z, \gamma), \\
A(\gamma; y', \beta') &= -A(\gamma; x', \alpha'), \\
S(a, y'; z, x') &= S(a, x'; z, y'), \\
S(a, z; \beta', x') &= -S(a, z; \alpha', y'), \\
S(a, y'; z, \alpha') &= -S(a, x'; z, \beta'), \\
S(a, y'; \gamma, x') &= -S(a, x'; \gamma, y'), \\
S(a, x'; \beta', z) &= -S(a, y'; \alpha', z), \\
S(a, \alpha'; \gamma, y') &= S(a, \beta'; \gamma, x'), \\
S(a, x'; \beta', \gamma) &= S(a, y'; \alpha', \gamma), \\
S(a, z; \alpha', \beta') &= S(a, z; \beta', \alpha'), \\
S(a, y'; \gamma, \alpha') &= S(a, x'; \gamma, \beta'), \\
S(a, \beta'; \gamma, \alpha') &= -S(a, \alpha'; \gamma, \beta'), \\
S(y', \beta'; \gamma, z) &= S(x', \alpha'; \gamma, z), \\
S(y', z; \gamma, \beta') &= S(x', z; \gamma, \alpha'), \\
S(y', z; \beta', \gamma) &= S(x', z; \alpha', \gamma).
\end{aligned}$$

#### Appendix C. Spherical approximation: $f$ -orbitals

##### Appendix C.1. Cubic basis

Independent parameters:

$$U(a), U(x), U(a, x), U(x, y). \tag{C.1}$$

Dependent parameters:

$$U(\alpha) = U(a), \tag{C.2}$$

$$\begin{aligned}
U(a, \alpha) &= -\frac{8}{9}U(a) + \frac{8}{9}U(x) - \frac{7}{9}U(a, x) \\
&+ \frac{16}{9}U(x, y), \\
U(x, \alpha) &= U(a, x),
\end{aligned}$$

$$\begin{aligned}
U(x, \beta) &= -\frac{5}{6}U(a) + \frac{5}{6}U(x) - \frac{2}{3}U(a, x) \\
&+ \frac{5}{3}U(x, y), \\
U(y, \alpha) &= -\frac{5}{6}U(a) + \frac{5}{6}U(x) - \frac{2}{3}U(a, x) \\
&+ \frac{5}{3}U(x, y), \\
U(\alpha, \beta) &= -\frac{1}{18}U(a) + \frac{1}{18}U(x) + \frac{8}{9}U(a, x) \\
&+ \frac{2}{18}U(x, y), \\
J(a, x) &= -\frac{3}{4}U(a) + \frac{5}{4}U(x) - \frac{1}{2}U(a, x), \\
J(x, y) &= \frac{45}{64}U(a) - \frac{13}{64}U(x) - \frac{1}{2}U(x, y), \\
J(a, \alpha) &= \frac{17}{18}U(a) - \frac{4}{9}U(x) + \frac{7}{18}U(a, x) \\
&- \frac{8}{9}U(x, y), \\
J(x, \alpha) &= -\frac{3}{4}U(a) + \frac{5}{4}U(x) - \frac{1}{2}U(a, x), \\
J(y, \alpha) &= \frac{161}{192}U(a) - \frac{65}{192}U(x) + \frac{1}{3}U(a, x) \\
&- \frac{5}{6}U(x, y), \\
J(x, \beta) &= \frac{161}{192}U(a) - \frac{65}{192}U(x) + \frac{1}{3}U(a, x) \\
&- \frac{5}{6}U(x, y), \\
J(\alpha, \beta) &= -\frac{371}{576}U(a) + \frac{659}{576}U(x) - \frac{4}{9}U(a, x) \\
&- \frac{1}{18}U(x, y), \\
T(x; y, \beta) &= \frac{5}{4}\sqrt{\frac{5}{3}}U(a) - \frac{5}{4}\sqrt{\frac{5}{3}}U(x) + \sqrt{\frac{5}{3}}U(a, x) \\
&- \sqrt{\frac{5}{3}}U(x, y), \\
T(y; x, \alpha) &= \frac{5}{4}\sqrt{\frac{5}{3}}U(a) - \frac{5}{4}\sqrt{\frac{5}{3}}U(x) + \sqrt{\frac{5}{3}}U(a, x) \\
&- \sqrt{\frac{5}{3}}U(x, y), \\
T(\alpha; y, \beta) &= \frac{1}{6}\sqrt{\frac{5}{3}}U(a) - \frac{1}{6}\sqrt{\frac{5}{3}}U(x) + \frac{1}{3}\sqrt{\frac{5}{3}}U(a, x) \\
&- \frac{1}{3}\sqrt{\frac{5}{3}}U(x, y), \\
T(\beta; x, \alpha) &= \frac{1}{6}\sqrt{\frac{5}{3}}U(a) - \frac{1}{6}\sqrt{\frac{5}{3}}U(x) + \frac{1}{3}\sqrt{\frac{5}{3}}U(a, x) \\
&- \frac{1}{3}\sqrt{\frac{5}{3}}U(x, y), \\
A(y; x, \alpha) &= -\frac{13}{64}\sqrt{\frac{5}{3}}U(a) + \frac{13}{64}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{1}{2}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{2}\sqrt{\frac{5}{3}}U(x, y), \\
A(x; x, \beta) &= -\frac{13}{64}\sqrt{\frac{5}{3}}U(a) + \frac{13}{64}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{1}{2}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{2}\sqrt{\frac{5}{3}}U(x, y), \\
A(\beta; x, \alpha) &= -\frac{61}{192}\sqrt{\frac{5}{3}}U(a) + \frac{61}{192}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{1}{6}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{6}\sqrt{\frac{5}{3}}U(x, y), \\
A(\alpha; y, \beta) &= -\frac{61}{192}\sqrt{\frac{5}{3}}U(a) + \frac{61}{192}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{1}{6}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{6}\sqrt{\frac{5}{3}}U(x, y), \\
S(a, x; z, y) &= -\frac{1}{9}\sqrt{\frac{5}{3}}U(a) + \frac{1}{9}\sqrt{\frac{5}{3}}U(x), \\
S(a, x; \gamma, y) &= \frac{31}{48}U(a) - \frac{31}{48}U(x) + \frac{2}{3}U(a, x) \\
&- \frac{2}{3}U(x, y), \\
S(a, y; \gamma, x) &= -\frac{31}{48}U(a) + \frac{31}{48}U(x) - \frac{2}{3}U(a, x) \\
&+ \frac{2}{3}U(x, y), \\
S(a, x; \beta, z) &= \frac{31}{48}U(a) - \frac{31}{48}U(x) + \frac{2}{3}U(a, x) \\
&- \frac{2}{3}U(x, y), \\
S(x, \alpha; \beta, y) &= \frac{4096}{6250}U(a) - \frac{4096}{6250}U(x) + \frac{5}{6}U(a, x) \\
&- \frac{5}{6}U(x, y), \\
S(x, y; \alpha, \beta) &= \frac{1}{192}U(a) - \frac{1}{192}U(x) + \frac{1}{6}U(a, x) \\
&- \frac{1}{6}U(x, y), \\
S(x, y; \beta, \alpha) &= -\frac{9}{8}U(a) + \frac{9}{8}U(x) - U(a, x) \\
&+ U(x, y), \\
S(a, \alpha; \beta, z) &= \frac{77}{48}\sqrt{\frac{5}{3}}U(a) - \frac{77}{48}\sqrt{\frac{5}{3}}U(x) \\
&+ \frac{4}{27}\sqrt{5}U(a, x) - \frac{4}{27}\sqrt{5}U(x, y), \\
S(a, \alpha; \gamma, y) &= -\frac{77}{48}\sqrt{\frac{5}{3}}U(a) + \frac{77}{48}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{4}{27}\sqrt{5}U(a, x) + \frac{4}{27}\sqrt{5}U(x, y), \\
S(a, x; \gamma, \beta) &= -\frac{1}{3}\sqrt{\frac{5}{3}}U(a) + \frac{1}{3}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{2}{3}\sqrt{\frac{5}{3}}U(a, x) + \frac{2}{3}\sqrt{\frac{5}{3}}U(x, y),
\end{aligned}$$

$$S(a, y; \gamma, \alpha) = \frac{1}{3}\sqrt{\frac{5}{3}}U(a) - \frac{1}{3}\sqrt{\frac{5}{3}}U(x) + \frac{2}{3}\sqrt{\frac{5}{3}}U(a, x) - \frac{2}{3}\sqrt{\frac{5}{3}}U(x, y) .$$

### Appendix C.2. Axial basis

Independent parameters:

$$U(a), U(x), U(a, x), U(x, y) . \quad (C.3)$$

Dependent parameters:

$$\begin{aligned} U(\alpha) &= U(a) , \\ U(a, \alpha) &= -\frac{8}{9}U(a) + \frac{8}{9}U(x) - \frac{7}{9}U(a, x) + \frac{16}{9}U(x, y) , \\ U(x, \alpha) &= U(a, x) , \\ U(x, \beta) &= -\frac{5}{6}U(a) + \frac{5}{6}U(x) - \frac{2}{3}U(a, x) + \frac{5}{3}U(x, y) , \\ U(y, \alpha) &= -\frac{5}{6}U(a) + \frac{5}{6}U(x) - \frac{2}{3}U(a, x) + \frac{5}{3}U(x, y) , \\ U(\alpha, \beta) &= -\frac{1}{18}U(a) + \frac{1}{18}U(x) + \frac{8}{9}U(a, x) + \frac{2}{18}U(x, y) , \\ J(a, x) &= -\frac{3}{4}U(a) + \frac{5}{4}U(x) - \frac{1}{2}U(a, x) , \\ J(x, y) &= \frac{45}{64}U(a) - \frac{13}{64}U(x) - \frac{1}{2}U(x, y) , \\ J(a, \alpha) &= \frac{17}{18}U(a) - \frac{4}{9}U(x) + \frac{7}{18}U(a, x) - \frac{8}{9}U(x, y) , \\ J(x, \alpha) &= -\frac{3}{4}U(a) + \frac{5}{4}U(x) - \frac{1}{2}U(a, x) , \\ J(y, \alpha) &= \frac{161}{192}U(a) - \frac{65}{192}U(x) + \frac{1}{3}U(a, x) - \frac{5}{6}U(x, y) , \\ J(x, \beta) &= \frac{161}{192}U(a) - \frac{65}{192}U(x) + \frac{1}{3}U(a, x) - \frac{5}{6}U(x, y) , \\ J(\alpha, \beta) &= -\frac{371}{576}U(a) + \frac{659}{576}U(x) - \frac{4}{9}U(a, x) - \frac{1}{18}U(x, y) , \\ T(x, y; \beta) &= \frac{5}{4}\sqrt{\frac{5}{3}}U(a) - \frac{5}{4}\sqrt{\frac{5}{3}}U(x) + \sqrt{\frac{5}{3}}U(a, x) - \sqrt{\frac{5}{3}}U(x, y) , \end{aligned} \quad (C.4)$$

$$\begin{aligned} T(y; x, \alpha) &= \frac{5}{4}\sqrt{\frac{5}{3}}U(a) - \frac{5}{4}\sqrt{\frac{5}{3}}U(x) + \sqrt{\frac{5}{3}}U(a, x) - \sqrt{\frac{5}{3}}U(x, y) , \\ T(\alpha; y, \beta) &= \frac{1}{6}\sqrt{\frac{5}{3}}U(a) - \frac{1}{6}\sqrt{\frac{5}{3}}U(x) + \frac{1}{3}\sqrt{\frac{5}{3}}U(a, x) - \frac{1}{3}\sqrt{\frac{5}{3}}U(x, y) , \\ T(\beta; x, \alpha) &= \frac{1}{6}\sqrt{\frac{5}{3}}U(a) - \frac{1}{6}\sqrt{\frac{5}{3}}U(x) + \frac{1}{3}\sqrt{\frac{5}{3}}U(a, x) - \frac{1}{3}\sqrt{\frac{5}{3}}U(x, y) , \\ A(y; x, \alpha) &= -\frac{13}{64}\sqrt{\frac{5}{3}}U(a) + \frac{13}{64}\sqrt{\frac{5}{3}}U(x) - \frac{1}{2}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{2}\sqrt{\frac{5}{3}}U(x, y) , \\ A(x; x, \beta) &= -\frac{13}{64}\sqrt{\frac{5}{3}}U(a) + \frac{13}{64}\sqrt{\frac{5}{3}}U(x) - \frac{1}{2}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{2}\sqrt{\frac{5}{3}}U(x, y) , \\ A(\beta; x, \alpha) &= -\frac{61}{192}\sqrt{\frac{5}{3}}U(a) + \frac{61}{192}\sqrt{\frac{5}{3}}U(x) - \frac{1}{6}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{6}\sqrt{\frac{5}{3}}U(x, y) , \\ A(\alpha; y, \beta) &= -\frac{61}{192}\sqrt{\frac{5}{3}}U(a) + \frac{61}{192}\sqrt{\frac{5}{3}}U(x) - \frac{1}{6}\sqrt{\frac{5}{3}}U(a, x) + \frac{1}{6}\sqrt{\frac{5}{3}}U(x, y) , \\ S(a, x; z, y) &= -\frac{1}{9}\sqrt{\frac{5}{3}}U(a) + \frac{1}{9}\sqrt{\frac{5}{3}}U(x) , \\ S(a, x; \gamma, y) &= \frac{31}{48}U(a) - \frac{31}{48}U(x) + \frac{2}{3}U(a, x) - \frac{2}{3}U(x, y) , \\ S(a, y; \gamma, x) &= -\frac{31}{48}U(a) + \frac{31}{48}U(x) - \frac{2}{3}U(a, x) + \frac{2}{3}U(x, y) , \\ S(a, x; \beta, z) &= \frac{31}{48}U(a) - \frac{31}{48}U(x) + \frac{2}{3}U(a, x) - \frac{2}{3}U(x, y) , \\ S(x, \alpha; \beta, y) &= \frac{4096}{6250}U(a) - \frac{4096}{6250}U(x) + \frac{5}{6}U(a, x) - \frac{5}{6}U(x, y) , \\ S(x, y; \alpha, \beta) &= \frac{1}{192}U(a) - \frac{1}{192}U(x) + \frac{1}{6}U(a, x) - \frac{1}{6}U(x, y) , \end{aligned}$$

$$\begin{aligned}
S(x, y; \beta, \alpha) &= -\frac{9}{8}U(a) + \frac{9}{8}U(x) - U(a, x) \\
&+ U(x, y) , \\
S(a, \alpha; \beta, z) &= \frac{77}{48}\sqrt{\frac{5}{3}}U(a) - \frac{77}{48}\sqrt{\frac{5}{3}}U(x) \\
&+ \frac{4}{27}\sqrt{5}U(a, x) - \frac{4}{27}\sqrt{5}U(x, y) , \\
S(a, \alpha; \gamma, y) &= -\frac{77}{48}\sqrt{\frac{5}{3}}U(a) + \frac{77}{48}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{4}{27}\sqrt{5}U(a, x) + \frac{4}{27}\sqrt{5}U(x, y) , \\
S(a, x; \gamma, \beta) &= -\frac{1}{3}\sqrt{\frac{5}{3}}U(a) + \frac{1}{3}\sqrt{\frac{5}{3}}U(x) \\
&- \frac{2}{3}\sqrt{\frac{5}{3}}U(a, x) + \frac{2}{3}\sqrt{\frac{5}{3}}U(x, y) , \\
S(a, y; \gamma, \alpha) &= \frac{1}{3}\sqrt{\frac{5}{3}}U(a) - \frac{1}{3}\sqrt{\frac{5}{3}}U(x) + \frac{2}{3}\sqrt{\frac{5}{3}}U(a, x) \\
&- \frac{2}{3}\sqrt{\frac{5}{3}}U(x, y) .
\end{aligned}$$

#### Appendix D. First order correction to the spherical approximation

##### Appendix D.1. d-orbitals, group $T_h$

Independent parameter variations:

$$\delta U(\zeta), \delta U(u, \zeta), \delta U(\zeta, \eta) . \quad (D.1)$$

Dependent parameter variations:

$$\begin{aligned}
\delta U(v, \eta) &= \frac{3}{4}\delta U(u, \zeta) , \\
\delta J(v, \zeta) &= \frac{1}{4}\delta U(\zeta) , \\
\delta J(v, \eta) &= \frac{1}{4}\delta U(\zeta) - \frac{3}{8}\delta U(u, \zeta) , \\
\delta J(u, \zeta) &= \frac{1}{4}\delta U(\zeta) - \frac{1}{2}\delta U(u, \zeta) , \\
\delta J(\zeta, \eta) &= \frac{1}{2}\delta U(\zeta) - \frac{1}{2}\delta U(\zeta, \eta) , \\
\delta S(v, \zeta; \xi, \eta) &= -\frac{27}{16}\delta U(u, \zeta) + \frac{3}{4}\delta U(\zeta, \eta) .
\end{aligned} \quad (D.2)$$

##### Appendix D.2. d-orbitals, group $D_{6h}$

Independent parameter variations:

$$\delta U(u), \delta U(\eta), \delta U(u, \zeta), \delta U(\eta, \xi), \delta U(v, \eta), \delta U(u, \eta) . \quad (D.3)$$

Dependent parameter variations:

$$\begin{aligned}
\delta U(v, \xi) &= \delta U(v, \eta) , \\
\delta J(v, u) &= \frac{1}{4}\delta U(u) , \\
\delta J(v, \eta) &= \frac{1}{4}\delta U(\eta) - \frac{1}{2}\delta U(v, \eta) ,
\end{aligned} \quad (D.4)$$

$$\begin{aligned}
\delta J(v, \xi) &= \frac{1}{4}\delta U(\eta) - \frac{1}{2}\delta U(v, \eta) , \\
\delta J(u, \eta) &= \frac{1}{4}\delta U(u) + \frac{1}{4}\delta U(\eta) - \frac{1}{2}\delta U(u, \eta) , \\
\delta T(\eta; v, u) &= -\frac{\sqrt{3}}{2}\delta U(u, \zeta) + \sqrt{3}\delta U(\eta, \xi) \\
&- \frac{3}{2}\sqrt{3}\delta U(v, \eta) - \frac{\sqrt{3}}{2}\delta U(u, \eta) , \\
\delta A(\eta; v, u) &= \frac{\sqrt{3}}{4}\delta U(u, \zeta) - \frac{\sqrt{3}}{2}\delta U(\eta, \xi) \\
&+ 3\frac{\sqrt{3}}{4}\delta U(v, \eta) + \frac{\sqrt{3}}{4}\delta U(u, \eta) , \\
\delta S(v, \zeta; \eta, \xi) &= -\frac{3}{4}\delta U(u, \zeta) + \frac{3}{2}\delta U(\eta, \xi) - \frac{9}{4}\delta U(v, \eta) \\
&- \frac{3}{4}\delta U(u, \eta) .
\end{aligned}$$

##### Appendix D.3. d-orbitals, group $D_{4h}$

Independent parameter variations:

$$\delta U(\eta), \delta U(u), \delta U(\zeta), \delta U(u, \zeta), \delta U(v, \eta), \delta U(u, \eta), \delta U(\zeta, \eta), \delta U(\eta, \xi), \delta T(\eta; v, u); . \quad (D.5)$$

Dependent parameter variations:

$$\begin{aligned}
\delta J(v, u) &= \frac{1}{4}\delta U(u) , \\
\delta J(v, \zeta) &= \frac{1}{4}\delta U(\zeta) , \\
\delta J(v, \eta) &= \frac{1}{4}\delta U(\eta) - \frac{1}{2}\delta U(v, \eta) , \\
\delta J(u, \zeta) &= \frac{1}{4}\delta U(u) + \frac{1}{4}\delta U(\zeta) - \frac{1}{2}\delta U(u, \zeta) , \\
\delta J(u, \eta) &= \frac{1}{4}\delta U(\eta) + \frac{1}{4}\delta U(u) - \frac{1}{2}\delta U(u, \eta) , \\
\delta J(\zeta, \eta) &= \frac{1}{4}\delta U(\eta) + \frac{1}{4}\delta U(\zeta) - \frac{1}{2}\delta U(\zeta, \eta) , \\
\delta J(\eta, \xi) &= \frac{1}{2}\delta U(\eta) - \frac{1}{2}\delta U(\eta, \xi) , \\
\delta A(\eta; v, u) &= -\frac{1}{2}\delta T(\eta; v, u) , \\
\delta S(v, \zeta; \xi, \eta) &= -\frac{3}{8}\delta U(u, \zeta) - \frac{7}{8}\delta U(v, \eta) - \frac{3}{8}\delta U(u, \eta) \\
&+ \frac{1}{4}\delta U(\zeta, \eta) + \frac{1}{2}\delta U(\eta, \xi) - 3\frac{\sqrt{3}}{4}\delta T(\eta; v, u) , \\
\delta S(u, \zeta; \eta, \xi) &= -\frac{\sqrt{3}}{4}\delta U(u, \zeta) - \frac{\sqrt{3}}{4}\delta U(v, \eta) \\
&+ \frac{\sqrt{3}}{4}\delta U(\zeta, \eta) - \frac{1}{2}\delta T(\eta; v, u) , \\
\delta S(u, \eta; \xi, \zeta) &= \frac{\sqrt{3}}{2}\delta U(u, \zeta) + \frac{\sqrt{3}}{2}\delta U(v, \eta) \\
&- \frac{\sqrt{3}}{2}\delta U(\zeta, \eta) + \delta T(\eta; v, u) .
\end{aligned} \quad (D.6)$$



Appendix D.4. *f*-orbitals, groups  $O_h$ ,  $O$ ,  $T_d$ 

Independent parameter variations:

$$\delta U(\alpha), \delta U(a, \alpha), \delta U(x, \alpha), \delta U(x, \beta), \delta U(\alpha, \beta), \quad (D.7)$$

$$\delta J(a, x), \delta J(x, y), \delta J(\alpha, \beta) .$$

Dependent parameter variations:

$$\delta J(a, \alpha) = \frac{1}{4}\delta U(\alpha) - \frac{1}{2}\delta U(a, \alpha) , \quad (D.8)$$

$$\delta J(x, \alpha) = -\frac{1}{60}\delta U(\alpha) - \frac{1}{2}\delta U(x, \alpha) + \frac{4}{5}\delta U(\alpha, \beta) \\ - \frac{8}{15}\delta J(x, y) + \frac{8}{15}\delta J(\alpha, \beta) ,$$

$$\delta J(y, \alpha) = \frac{7}{30}\delta U(\alpha) - \frac{1}{2}\delta U(x, \beta) + \frac{1}{60}\delta U(\alpha, \beta) \\ + \frac{3}{10}\delta J(x, y) + \frac{1}{30}\delta J(\alpha, \beta) ,$$

$$\delta T(y; x, \alpha) = \frac{2}{5\sqrt{15}}\delta U(\alpha) + \frac{9}{4}\sqrt{\frac{3}{5}}\delta U(x, \alpha) \\ - \frac{3}{8}\sqrt{\frac{3}{5}}\delta U(x, \beta) - \frac{257}{80\sqrt{15}}\delta U(\alpha, \beta) + 2\sqrt{\frac{3}{5}}\delta J(x, y) \\ - \frac{4}{5\sqrt{15}}\delta J(\alpha, \beta) ,$$

$$\delta T(\beta; x, \alpha) = -\frac{1}{4\sqrt{15}}\delta U(x, \alpha) - \frac{13}{8\sqrt{15}}\delta U(x, \beta) \\ + \frac{1}{9}\sqrt{\frac{5}{3}}\delta U(\alpha, \beta) - \frac{2}{3\sqrt{15}}\delta J(x, y) ,$$

$$\delta A(x; x, \beta) = \frac{1}{40\sqrt{15}}\delta U(\alpha) - \frac{9}{8}\sqrt{\frac{3}{5}}\delta U(x, \alpha) \\ + \frac{3}{16}\sqrt{\frac{3}{5}}\delta U(x, \beta) + \frac{221}{800}\sqrt{\frac{3}{5}}\delta U(\alpha, \beta) - \frac{1}{4}\sqrt{\frac{3}{5}}\delta J(x, y) \\ - \frac{1}{20\sqrt{15}}\delta J(\alpha, \beta) ,$$

$$\delta A(\beta; x, \alpha) = -\frac{1}{8}\sqrt{\frac{3}{5}}\delta U(\alpha) + \frac{1}{8\sqrt{15}}\delta U(x, \alpha) \\ + \frac{13}{16\sqrt{15}}\delta U(x, \beta) - \frac{1}{32}\sqrt{\frac{3}{5}}\delta U(\alpha, \beta) - \frac{1}{12\sqrt{15}}\delta J(x, y) \\ + \frac{1}{4}\sqrt{\frac{3}{5}}\delta J(\alpha, \beta) ,$$

$$\delta S(a, x; z, y) = \frac{1}{8}\sqrt{\frac{3}{5}}\delta J(a, x) - \frac{4}{5\sqrt{15}}\delta J(x, y) ,$$

$$\delta S(a, x; \beta, z) = \frac{1}{30}\delta U(\alpha) - \frac{3}{16}\delta U(a, \alpha) + \frac{79}{160}\delta U(x, \alpha) \\ + \frac{7}{320}\delta U(x, \beta) - \frac{379}{1920}\delta U(\alpha, \beta) - \frac{1}{8}\delta J(a, x) \\ + \frac{73}{180}\delta J(x, y) - \frac{1}{15}\delta J(\alpha, \beta) ,$$

$$\delta S(a, x; \gamma, \beta) = \frac{1}{9}\sqrt{\frac{5}{3}}\delta U(a, \alpha) + \frac{1}{32\sqrt{15}}\delta U(x, \alpha) \\ + \frac{73}{64\sqrt{15}}\delta U(x, \beta) - \frac{9\sqrt{15}}{128}\delta U(\alpha, \beta) + \frac{1}{12\sqrt{15}}\delta J(x, y) ,$$

$$\delta S(a, \alpha; \beta, z) = \frac{1}{\sqrt{15}}\delta U(\alpha) - \frac{1}{8\sqrt{15}}\delta U(a, \alpha) \\ - \frac{1}{16\sqrt{15}}\delta U(x, \alpha) - \frac{73}{32\sqrt{15}}\delta U(x, \beta) + \frac{71}{64\sqrt{15}}\delta U(\alpha, \beta) \\ - \frac{1}{8\sqrt{15}}\delta J(a, x) + \frac{1}{2\sqrt{15}}\delta J(x, y) - \frac{2}{\sqrt{15}}\delta J(\alpha, \beta) ,$$

$$\delta S(x, y; \alpha, \beta) = -\frac{1}{60}\delta U(\alpha) + \frac{1}{10}\delta U(x, \alpha) \\ - \frac{1}{10}\delta U(x, \beta) + \frac{1}{60}\delta U(\alpha, \beta) - \frac{1}{18}\delta J(x, y) \\ + \frac{1}{30}\delta J(\alpha, \beta) ,$$

$$\delta S(x, y; \beta, \alpha) = -\frac{2}{15}\delta U(\alpha) - \frac{3}{5}\delta U(x, \alpha) + \frac{3}{5}\delta U(x, \beta) \\ + \frac{2}{15}\delta U(\alpha, \beta) - \frac{4}{9}\delta J(x, y) + \frac{4}{5}\delta J(\alpha, \beta) ,$$

$$\delta S(x, \alpha; \beta, y) = \frac{1}{20}\delta U(\alpha) + \frac{1}{2}\delta U(x, \alpha) - \frac{1}{2}\delta U(x, \beta) \\ - \frac{1}{20}\delta U(\alpha, \beta) + \frac{1}{6}\delta J(x, y) - \frac{1}{10}\delta J(\alpha, \beta) .$$

Appendix D.5. *f*-orbitals, group  $T_h$ 

Independent parameter variations:

$$\delta U(\alpha), \delta U(a, \alpha), \delta U(x, \alpha), \delta U(x, \beta), \delta U(\alpha, \beta), \quad (D.9)$$

$$\delta J(a, x), \delta J(x, y), \delta J(\alpha, \beta) .$$

Dependent parameter variations:

$$\delta U(y, \alpha) = \delta U(x, \beta) , \quad (D.10)$$

$$\delta J(a, \alpha) = \frac{1}{4}\delta U(\alpha) - \frac{1}{2}\delta U(a, \alpha) ,$$

$$\delta J(x, \alpha) = -\frac{1}{60}\delta U(\alpha) - \frac{1}{2}\delta U(x, \alpha) + \frac{4}{5}\delta U(\alpha, \beta) \\ - \frac{8}{15}\delta J(x, y) + \frac{8}{15}\delta J(\alpha, \beta) ,$$

$$\delta J(x, \beta) = \frac{7}{30}\delta U(\alpha) - \frac{1}{2}\delta U(x, \beta) + \frac{1}{60}\delta U(\alpha, \beta) \\ + \frac{3}{10}\delta J(x, y) + \frac{1}{30}\delta J(\alpha, \beta) ,$$

$$\delta J(y, \alpha) = \frac{7}{30}\delta U(\alpha) - \frac{1}{2}\delta U(x, \beta) + \frac{1}{60}\delta U(\alpha, \beta) \\ + \frac{3}{10}\delta J(x, y) + \frac{1}{30}\delta J(\alpha, \beta) ,$$

$$\delta T(y; x, \alpha) = \frac{2}{5\sqrt{15}}\delta U(\alpha) + \frac{9}{4}\sqrt{\frac{3}{5}}\delta U(x, \alpha) \\ - \frac{3}{8}\sqrt{\frac{3}{5}}\delta U(x, \beta) - \frac{257}{80\sqrt{15}}\delta U(\alpha, \beta) + 2\sqrt{\frac{3}{5}}\delta J(x, y) \\ - \frac{4}{5\sqrt{15}}\delta J(\alpha, \beta) ,$$

$$\delta T(x; y, \beta) = \frac{2}{5\sqrt{15}}\delta U(\alpha) + \frac{9}{4}\sqrt{\frac{3}{5}}\delta U(x, \alpha) \\ - \frac{3}{8}\sqrt{\frac{3}{5}}\delta U(x, \beta) - \frac{257}{80\sqrt{15}}\delta U(\alpha, \beta) + 2\sqrt{\frac{3}{5}}\delta J(x, y)$$

$$\begin{aligned}
& -\frac{4}{5\sqrt{15}}\delta J(\alpha, \beta), \\
\delta T(\beta; x, \alpha) &= -\frac{1}{4\sqrt{15}}\delta U(x, \alpha) - \frac{13}{8\sqrt{15}}\delta U(x, \beta) \\
& + \frac{1}{9}\sqrt{\frac{5}{3}}\delta U(\alpha, \beta) - \frac{2}{3\sqrt{15}}\delta J(x, y), \\
\delta T(\alpha; y, \beta) &= -\frac{1}{4\sqrt{15}}\delta U(x, \alpha) - \frac{13}{8\sqrt{15}}\delta U(x, \beta) \\
& + \frac{1}{9}\sqrt{\frac{5}{3}}\delta U(\alpha, \beta) - \frac{2}{3\sqrt{15}}\delta J(x, y), \\
\delta A(x; x, \beta) &= \frac{1}{40\sqrt{15}}\delta U(\alpha) - \frac{9}{8}\sqrt{\frac{3}{5}}\delta U(x, \alpha) \\
& + \frac{3}{16}\sqrt{\frac{3}{5}}\delta U(x, \beta) + \frac{221}{800}\sqrt{\frac{3}{5}}\delta U(\alpha, \beta) - \frac{1}{4}\sqrt{\frac{3}{5}}\delta J(x, y) \\
& - \frac{1}{20\sqrt{15}}\delta J(\alpha, \beta), \\
\delta A(y; x, \alpha) &= \frac{1}{40\sqrt{15}}\delta U(\alpha) - \frac{9}{8}\sqrt{\frac{3}{5}}\delta U(x, \alpha) \\
& + \frac{3}{16}\sqrt{\frac{3}{5}}\delta U(x, \beta) + \frac{221}{800}\sqrt{\frac{3}{5}}\delta U(\alpha, \beta) - \frac{1}{4}\sqrt{\frac{3}{5}}\delta J(x, y) \\
& - \frac{1}{20\sqrt{15}}\delta J(\alpha, \beta), \\
\delta A(\beta; x, \alpha) &= -\frac{1}{8}\sqrt{\frac{3}{5}}\delta U(\alpha) + \frac{1}{8\sqrt{15}}\delta U(x, \alpha) \\
& + \frac{13}{16\sqrt{15}}\delta U(x, \beta) - \frac{1}{32}\sqrt{\frac{3}{5}}\delta U(\alpha, \beta) - \frac{1}{12\sqrt{15}}\delta J(x, y) \\
& + \frac{1}{4}\sqrt{\frac{3}{5}}\delta J(\alpha, \beta), \\
\delta A(\alpha; y, \beta) &= -\frac{1}{8}\sqrt{\frac{3}{5}}\delta U(\alpha) + \frac{1}{8\sqrt{15}}\delta U(x, \alpha) \\
& + \frac{13}{16\sqrt{15}}\delta U(x, \beta) - \frac{1}{32}\sqrt{\frac{3}{5}}\delta U(\alpha, \beta) - \frac{1}{12\sqrt{15}}\delta J(x, y) \\
& + \frac{1}{4}\sqrt{\frac{3}{5}}\delta J(\alpha, \beta), \\
\delta S(a, x; z, y) &= \frac{1}{8}\sqrt{\frac{3}{5}}\delta J(a, x) - \frac{4}{5\sqrt{15}}\delta J(x, y), \\
\delta S(a, x; \gamma, y) &= \frac{1}{30}\delta U(\alpha) - \frac{3}{16}\delta U(a, \alpha) + \frac{79}{160}\delta U(x, \alpha) \\
& + \frac{7}{320}\delta U(x, \beta) - \frac{379}{1920}\delta U(\alpha, \beta) - \frac{1}{8}\delta J(a, x) \\
& + \frac{73}{180}\delta J(x, y) - \frac{1}{15}\delta J(\alpha, \beta), \\
\delta S(a, x; \gamma, \beta) &= \frac{1}{9}\sqrt{\frac{5}{3}}\delta U(a, \alpha) + \frac{1}{32\sqrt{15}}\delta U(x, \alpha) \\
& + \frac{73}{64\sqrt{15}}\delta U(x, \beta) - \frac{9\sqrt{15}}{128}\delta U(\alpha, \beta) + \frac{1}{12\sqrt{15}}\delta J(x, y), \\
\delta S(a, y; \gamma, x) &= -\frac{1}{30}\delta U(\alpha) + \frac{3}{16}\delta U(a, \alpha)
\end{aligned}$$

$$\begin{aligned}
& -\frac{79}{160}\delta U(x, \alpha) - \frac{7}{320}\delta U(x, \beta) + \frac{379}{1920}\delta U(\alpha, \beta) \\
& + \frac{1}{8}\delta J(a, x) - \frac{73}{180}\delta J(x, y) + \frac{1}{15}\delta J(\alpha, \beta), \\
\delta S(a, y; \gamma, \alpha) &= -\frac{1}{9}\sqrt{\frac{5}{3}}\delta U(a, \alpha) - \frac{1}{32\sqrt{15}}\delta U(x, \alpha) \\
& - \frac{73}{64\sqrt{15}}\delta U(x, \beta) + \frac{9\sqrt{15}}{128}\delta U(\alpha, \beta) - \frac{1}{12\sqrt{15}}\delta J(x, y), \\
\delta S(a, \alpha; \gamma, y) &= -\frac{1}{\sqrt{15}}\delta U(\alpha) + \frac{1}{8\sqrt{15}}\delta U(a, \alpha) \\
& + \frac{1}{16\sqrt{15}}\delta U(x, \alpha) + \frac{73}{32\sqrt{15}}\delta U(x, \beta) - \frac{71}{64\sqrt{15}}\delta U(\alpha, \beta) \\
& + \frac{1}{8\sqrt{15}}\delta J(a, x) - \frac{1}{2\sqrt{15}}\delta J(x, y) + \frac{2}{\sqrt{15}}\delta J(\alpha, \beta), \\
\delta S(x, y; \alpha, \beta) &= -\frac{1}{60}\delta U(\alpha) + \frac{1}{10}\delta U(x, \alpha) \\
& - \frac{1}{10}\delta U(x, \beta) + \frac{1}{60}\delta U(\alpha, \beta) - \frac{1}{18}\delta J(x, y) \\
& + \frac{1}{30}\delta J(\alpha, \beta), \\
\delta S(x, y; \beta, \alpha) &= -\frac{2}{15}\delta U(\alpha) - \frac{3}{5}\delta U(x, \alpha) + \frac{3}{5}\delta U(x, \beta) \\
& + \frac{2}{15}\delta U(\alpha, \beta) - \frac{4}{9}\delta J(x, y) + \frac{4}{5}\delta J(\alpha, \beta), \\
\delta S(x, \alpha; \beta, y) &= \frac{1}{20}\delta U(\alpha) + \frac{1}{2}\delta U(x, \alpha) - \frac{1}{2}\delta U(x, \beta) \\
& - \frac{1}{20}\delta U(\alpha, \beta) + \frac{1}{6}\delta J(x, y) - \frac{1}{10}\delta J(\alpha, \beta).
\end{aligned}$$

#### Appendix D.6. *f*-orbitals, group $D_{6h}$

Independent parameter variations:

$$\begin{aligned}
& \delta U(z), \delta U(\alpha'), \delta U(\beta'), \delta U(x', y'), \delta U(x', z), \quad (D.11) \\
& \delta U(a, \alpha'), \delta U(x', \alpha'), \delta U(a, \beta'), \delta U(a, \gamma), \delta U(x', \beta'), \\
& \delta U(z, \alpha'), \delta U(\alpha', \beta'), \delta J(x', \alpha'), \delta J(a, x'), \delta J(a, \alpha'), \\
& \delta J(a, z).
\end{aligned}$$

Dependent parameter variations:

$$\begin{aligned}
\delta U(z, \beta') &= \frac{1}{6}\delta U(z) - \frac{73}{150}\delta U(\alpha') - \frac{8}{15}\delta J(x', \alpha') \quad (D.12) \\
& - \frac{7}{6}\delta U(x', y') + \frac{16}{25}\delta U(a, \alpha') - \frac{11}{30}\delta U(x', \alpha') \\
& - \frac{3}{5}\delta U(a, \beta') - \frac{1}{15}\delta U(a, \gamma) + \frac{3}{2}\delta U(x', \beta') \\
& + \frac{3}{5}\delta U(z, \alpha') + \frac{1}{10}\delta U(\alpha', \beta') - \frac{106}{45}\delta J(a, x') \\
& + \frac{62}{25}\delta J(a, \alpha') - \frac{2}{3}\delta J(a, z), \\
\delta J(a, y') &= \delta J(a, x'), \\
\delta J(a, \beta') &= -\frac{1}{4}\delta U(\alpha') + \frac{1}{4}\delta U(\beta') + \frac{1}{2}\delta U(a, \alpha') \\
& - \frac{1}{2}\delta U(a, \beta') + \delta J(a, \alpha'), \\
\delta J(x', z) &= \frac{1}{4}\delta U(z) + \frac{1}{8}\delta U(\alpha') - \frac{1}{2}\delta U(x', z)
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{4}\delta U(a, \alpha') + \frac{5}{6}\delta J(a, x') - \frac{1}{2}\delta J(a, \alpha') , \\
& \delta J(x', \beta') = \frac{1}{2}\delta U(z) - \frac{171}{100}\delta U(\alpha') + \frac{1}{4}\delta U(\beta') \\
& -\frac{3}{5}\delta J(x', \alpha') - \frac{7}{2}\delta U(x', y') + \frac{48}{25}\delta U(a, \alpha') \\
& +\frac{12}{5}\delta U(x', \alpha') - \frac{9}{5}\delta U(a, \beta') - \frac{2}{10}\delta U(a, \gamma) \\
& +\delta U(x', \beta') - \frac{6}{5}\delta U(z, \alpha') + \frac{3}{10}\delta U(\alpha', \beta') \\
& -\frac{106}{15}\delta J(a, x') + \frac{186}{25}\delta J(a, \alpha') - 2\delta J(a, z) , \\
& \delta J(z, \alpha') = \frac{5}{8}\delta U(z) - \frac{17}{10}\delta U(\alpha') + \frac{3}{2}\delta J(x', \alpha') \\
& +\frac{63}{20}\delta U(a, \alpha') + \frac{3}{4}\delta U(x', \alpha') - \frac{1}{2}\delta U(z, \alpha') \\
& -\frac{13}{2}\delta J(a, x') + \frac{63}{10}\delta J(a, \alpha') - \frac{3}{2}\delta J(a, z) , \\
& \delta J(z, \beta') = \frac{31}{24}\delta U(z) - \frac{1169}{300}\delta U(\alpha') + \frac{1}{4}\delta U(\beta') \\
& -\frac{19}{30}\delta J(x', \alpha') - \frac{14}{3}\delta U(x', y') + \frac{571}{100}\delta U(a, \alpha') \\
& +\frac{227}{60}\delta U(x', \alpha') - \frac{12}{5}\delta U(a, \beta') - \frac{4}{5}\delta U(a, \gamma) \\
& +\frac{3}{2}\delta U(x', \beta') - \frac{21}{10}\delta U(z, \alpha') + \frac{2}{5}\delta U(\alpha', \beta') \\
& -\frac{1433}{90}\delta J(a, x') + \frac{811}{50}\delta J(a, \alpha') - \frac{25}{6}\delta J(a, z) , \\
& \delta J(\alpha', \beta') = \frac{1}{4}\delta U(\alpha') + \frac{1}{4}\delta U(\beta') - \frac{1}{2}\delta U(\alpha', \beta') , \\
& \delta T(a; x', \alpha') = -\frac{\sqrt{\frac{5}{3}}}{4}\delta U(z) + \frac{151}{40\sqrt{15}}\delta U(\alpha') \\
& +2\sqrt{\frac{3}{5}}\delta J(x', \alpha') + \frac{2}{3}\sqrt{\frac{5}{3}}\delta U(x', y') - \frac{29}{5\sqrt{15}}\delta U(a, \alpha') \\
& -\frac{19}{4\sqrt{15}}\delta U(x', \alpha') + \frac{1}{6}\sqrt{\frac{5}{3}}\delta U(a, \gamma) + \sqrt{\frac{3}{5}}\delta U(z, \alpha') \\
& +\frac{43}{3\sqrt{15}}\delta J(a, x') - \frac{83}{5\sqrt{15}}\delta J(a, \alpha') + \sqrt{\frac{5}{3}}\delta J(a, z) , \\
& \delta T(a; y', \beta') = -\frac{1}{8\sqrt{15}}\delta U(\alpha') + \frac{1}{2}\sqrt{\frac{5}{3}}\delta J(x', \alpha') \\
& +\frac{13\sqrt{\frac{5}{3}}}{12}\delta U(x', y') + \frac{7}{2\sqrt{15}}\delta U(a, \alpha') - \frac{1}{2}\sqrt{\frac{5}{3}}\delta U(x', \alpha') \\
& +\frac{2}{\sqrt{15}}\delta U(a, \beta') - \frac{1}{3\sqrt{15}}\delta U(a, \gamma) - \frac{\sqrt{\frac{5}{3}}}{4}\delta U(x', \beta') \\
& -\frac{1}{4}\sqrt{\frac{3}{5}}\delta U(\alpha', \beta') + \frac{2}{3}\sqrt{\frac{5}{3}}\delta J(a, x') - \frac{2}{\sqrt{15}}\delta J(a, \alpha') , \\
& \delta T(y'; x', \alpha') = -\frac{9\sqrt{\frac{3}{5}}}{20}\delta U(\alpha') - \frac{1}{\sqrt{15}}\delta J(x', \alpha')
\end{aligned}$$

$$\begin{aligned}
& +\frac{16}{5\sqrt{15}}\delta U(a, \alpha') - \frac{1}{2\sqrt{15}}\delta U(x', \alpha') - \frac{32}{3\sqrt{15}}\delta J(a, x') \\
& +\frac{32}{5\sqrt{15}}\delta J(a, \alpha') , \\
& \delta T(x'; y', \beta') = \frac{1}{2\sqrt{15}}\delta U(z) - \frac{11}{100\sqrt{15}}\delta U(\alpha') \\
& -\frac{\sqrt{\frac{3}{5}}}{5}\delta J(x', \alpha') - \frac{7}{2\sqrt{15}}\delta U(x', y') - \frac{32}{25\sqrt{15}}\delta U(a, \alpha') \\
& +\frac{4\sqrt{\frac{3}{5}}}{5}\delta U(x', \alpha') - \frac{3\sqrt{\frac{3}{5}}}{5}\delta U(a, \beta') - \frac{1}{5\sqrt{15}}\delta U(a, \gamma) \\
& +2\sqrt{\frac{3}{5}}\delta U(x', \beta') - \frac{2\sqrt{\frac{3}{5}}}{5}\delta U(z, \alpha') + \frac{\sqrt{\frac{3}{5}}}{10}\delta U(\alpha', \beta') \\
& +\frac{6\sqrt{\frac{3}{5}}}{5}\delta J(a, x') + \frac{26}{25\sqrt{15}}\delta J(a, \alpha') - \frac{2}{\sqrt{15}}\delta J(a, z) , \\
& \delta T(x'; z, \gamma) = \frac{\sqrt{\frac{5}{3}}}{4}\delta U(z) - \frac{161}{80\sqrt{15}}\delta U(\alpha') \\
& +\frac{1}{4}\sqrt{\frac{3}{5}}\delta J(x', \alpha') + \frac{1}{3}\sqrt{\frac{5}{3}}\delta U(x', y') - \frac{\sqrt{\frac{5}{3}}}{4}\delta U(x', z) \\
& +\frac{73}{20\sqrt{15}}\delta U(a, \alpha') + \frac{7\sqrt{\frac{3}{5}}}{8}\delta U(x', \alpha') + \frac{\sqrt{\frac{5}{3}}}{12}\delta U(a, \gamma) \\
& -\frac{3}{4}\sqrt{\frac{3}{5}}\delta U(z, \alpha') - \frac{17}{6\sqrt{15}}\delta J(a, x') + \frac{73}{10\sqrt{15}}\delta J(a, \alpha') \\
& -\sqrt{\frac{5}{3}}\delta J(a, z) , \\
& \delta A(a; a, \alpha') = \frac{\sqrt{\frac{5}{3}}}{8}\delta U(z) - \frac{53}{40\sqrt{15}}\delta U(\alpha') \\
& +\frac{1}{2\sqrt{15}}\delta J(x', \alpha') - \frac{1}{3}\sqrt{\frac{5}{3}}\delta U(x', y') + \frac{23}{20\sqrt{15}}\delta U(a, \alpha') \\
& +\sqrt{\frac{3}{5}}\delta U(x', \alpha') - \frac{\sqrt{\frac{5}{3}}}{12}\delta U(a, \gamma) - 2\sqrt{\frac{3}{5}}\delta U(z, \alpha') \\
& -\frac{19}{3\sqrt{15}}\delta J(a, x') + \frac{8\sqrt{\frac{3}{5}}}{5}\delta J(a, \alpha') - \frac{1}{2}\sqrt{\frac{5}{3}}\delta J(a, z) , \\
& \delta A(a; a, \beta') = -\frac{\sqrt{\frac{5}{3}}}{8}\delta U(z) + \frac{53}{40\sqrt{15}}\delta U(\alpha') \\
& -\frac{1}{2\sqrt{15}}\delta J(x', \alpha') + \frac{1}{3}\sqrt{\frac{5}{3}}\delta U(x', y') - \frac{4\sqrt{\frac{3}{5}}}{5}\delta U(a, \alpha') \\
& -\frac{7}{4\sqrt{15}}\delta U(x', \alpha') + \frac{\sqrt{\frac{5}{3}}}{4}\delta U(a, \beta') + \frac{\sqrt{\frac{5}{3}}}{12}\delta U(a, \gamma) \\
& -\frac{\sqrt{\frac{5}{3}}}{4}\delta U(x', \beta') + 2\sqrt{\frac{3}{5}}\delta U(z, \alpha') + \frac{19}{3\sqrt{15}}\delta J(a, x')
\end{aligned}$$

$$\begin{aligned}
& -\frac{8\sqrt{\frac{3}{5}}}{5}\delta J(a, \alpha') + \frac{1}{2}\sqrt{\frac{5}{3}}\delta J(a, z), \\
\delta A(x'; x', \gamma) &= -\frac{\sqrt{15}}{32}\delta U(z) + \frac{53}{32\sqrt{15}}\delta U(\alpha') \\
& -\frac{1}{8}\sqrt{\frac{3}{5}}\delta J(x', \alpha') - \frac{1}{6}\sqrt{\frac{5}{3}}\delta U(x', y') + \frac{\sqrt{\frac{5}{3}}}{8}\delta U(x', z) \\
& -\frac{5\sqrt{\frac{5}{3}}}{8}\delta U(a, \alpha') - \frac{7}{16}\sqrt{\frac{3}{5}}\delta U(x', \alpha') - \frac{\sqrt{\frac{5}{3}}}{24}\delta U(a, \gamma) \\
& +\frac{3}{8}\sqrt{\frac{3}{5}}\delta U(z, \alpha') + \frac{77}{12\sqrt{15}}\delta J(a, x') - \frac{5}{4}\sqrt{\frac{5}{3}}\delta J(a, \alpha') \\
& +\frac{1}{8\sqrt{15}}\delta J(a, z), \\
\delta S(a, x'; z, \beta') &= -\frac{13}{96}\delta U(z) + \frac{181}{600}\delta U(\alpha') \\
& +\frac{1}{10}\delta J(x', \alpha') + \frac{7}{12}\delta U(x', y') - \frac{53}{150}\delta U(a, \alpha') \\
& -\frac{2}{5}\delta U(x', \alpha') + \frac{3}{10}\delta U(a, \beta') + \frac{1}{30}\delta U(a, \gamma) \\
& -\frac{1}{4}\delta U(x', \beta') + \frac{2}{10}\delta U(z, \alpha') - \frac{1}{20}\delta U(\alpha', \beta') \\
& +\frac{16}{15}\delta J(a, x') - \frac{98}{75}\delta J(a, \alpha') + \frac{13}{24}\delta J(a, z), \\
\delta S(a, x'; \beta', z) &= -\frac{1}{12}\delta U(z) + \frac{143}{2400}\delta U(\alpha') \\
& -\frac{7}{40}\delta J(x', \alpha') - \frac{1}{12}\delta U(x', y') + \frac{1}{8}\delta U(x', z) \\
& -\frac{199}{600}\delta U(a, \alpha') + \frac{11}{80}\delta U(x', \alpha') + \frac{2}{10}\delta U(a, \beta') \\
& +\frac{11}{120}\delta U(a, \gamma) - \frac{1}{4}\delta U(x', \beta') + \frac{1}{40}\delta U(z, \alpha') \\
& +\frac{1}{20}\delta U(\alpha', \beta') - \frac{7}{60}\delta J(a, x') - \frac{19}{300}\delta J(a, \alpha') \\
& +\frac{1}{3}\delta J(a, z), \\
\delta S(a, x'; \gamma, y') &= -\frac{3}{8}\delta U(z) + \frac{51}{50}\delta U(\alpha') \\
& -\frac{3}{10}\delta J(x', \alpha') - \frac{189}{100}\delta U(a, \alpha') - \frac{21}{20}\delta U(x', \alpha') \\
& +\frac{9}{10}\delta U(z, \alpha') + \frac{33}{10}\delta J(a, x') - \frac{189}{50}\delta J(a, \alpha') \\
& +\frac{3}{2}\delta J(a, z), \\
\delta S(a, y'; z, \alpha') &= \frac{5}{96}\delta U(z) - \frac{7}{120}\delta U(\alpha') + \frac{1}{6}\delta J(x', \alpha') \\
& +\frac{1}{30}\delta U(a, \alpha') + \frac{1}{12}\delta U(x', \alpha') + \frac{2}{18}\delta J(a, x') \\
& +\frac{1}{15}\delta J(a, \alpha') - \frac{5}{24}\delta J(a, z), \\
\delta S(a, y'; \alpha', z) &= \frac{1}{6}\delta U(z) - \frac{727}{2400}\delta U(\alpha') \\
& -\frac{11}{120}\delta J(x', \alpha') - \frac{1}{2}\delta U(x', y') - \frac{1}{8}\delta U(x', z)
\end{aligned}$$

$$\begin{aligned}
& +\frac{91}{600}\delta U(a, \alpha') + \frac{163}{240}\delta U(x', \alpha') - \frac{1}{8}\delta U(a, \gamma) \\
& -\frac{9}{40}\delta U(z, \alpha') - \frac{191}{180}\delta J(a, x') + \frac{391}{300}\delta J(a, \alpha') \\
& -\frac{2}{3}\delta J(a, z), \\
\delta S(a, z; \alpha', y') &= -\frac{1}{16}\delta U(z) + \frac{149}{800}\delta U(\alpha') \\
& +\frac{17}{40}\delta J(x', \alpha') + \frac{1}{2}\delta U(x', y') + \frac{1}{8}\delta U(x', z) \\
& -\frac{17}{200}\delta U(a, \alpha') - \frac{41}{80}\delta U(x', \alpha') + \frac{1}{8}\delta U(a, \gamma) \\
& +\frac{9}{40}\delta U(z, \alpha') + \frac{77}{60}\delta J(a, x') - \frac{117}{100}\delta J(a, \alpha') \\
& +\frac{1}{4}\delta J(a, z), \\
\delta S(a, z; \beta', x') &= -\frac{3}{16}\delta U(z) + \frac{87}{160}\delta U(\alpha') \\
& +\frac{3}{8}\delta J(x', \alpha') + \frac{5}{4}\delta U(x', y') - \frac{1}{8}\delta U(x', z) \\
& -\frac{3}{8}\delta U(a, \alpha') - \frac{15}{16}\delta U(x', \alpha') + \frac{2}{5}\delta U(a, \beta') \\
& -\frac{1}{40}\delta U(a, \gamma) - \frac{1}{4}\delta U(x', \beta') + \frac{3}{8}\delta U(z, \alpha') \\
& -\frac{3}{20}\delta U(\alpha', \beta') + \frac{9}{4}\delta J(a, x') - \frac{51}{20}\delta J(a, \alpha') \\
& +\frac{3}{4}\delta J(a, z), \\
\delta S(a, \alpha'; \gamma, \beta') &= -\frac{5}{24}\delta U(z) + \frac{29}{60}\delta U(\alpha') \\
& -\frac{1}{6}\delta J(x', \alpha') + \frac{5}{12}\delta U(x', y') - \frac{17}{15}\delta U(a, \alpha') \\
& -\frac{7}{12}\delta U(x', \alpha') - \frac{1}{4}\delta U(a, \beta') + \frac{2}{3}\delta U(a, \gamma) \\
& +\frac{1}{2}\delta U(z, \alpha') + \frac{1}{4}\delta U(\alpha', \beta') + \frac{43}{18}\delta J(a, x') \\
& -\frac{53}{30}\delta J(a, \alpha') \\
& +\frac{5}{6}\delta J(a, z), \\
\delta S(x', y'; \beta', \alpha') &= -\frac{1}{12}\delta U(z) + \frac{29}{150}\delta U(\alpha') \\
& -\frac{1}{15}\delta J(x', \alpha') - \frac{1}{3}\delta U(x', y') - \frac{34}{75}\delta U(a, \alpha') \\
& -\frac{7}{30}\delta U(x', \alpha') - \frac{1}{10}\delta U(a, \beta') - \frac{7}{30}\delta U(a, \gamma) \\
& +\frac{2}{10}\delta U(z, \alpha') + \frac{1}{10}\delta U(\alpha', \beta') + \frac{13}{45}\delta J(a, x') \\
& -\frac{53}{75}\delta J(a, \alpha') + \frac{1}{3}\delta J(a, z).
\end{aligned}$$

#### Appendix D.7. *f*-orbitals, group $D_{4h}$

Independent parameter variations:

$$\begin{aligned}
& \delta U(z), \delta U(\alpha'), \delta U(\gamma), \delta U(x', y'), \delta U(x', z), \\
& \delta U(a, \alpha'), \delta U(x', \alpha'), \delta U(a, \gamma), \delta U(z, \alpha'), \delta U(x', \gamma),
\end{aligned} \tag{D.13}$$

$$\delta U(z, \gamma), \delta U(\alpha', \beta'), \delta J(x', \gamma), \delta J(x', \alpha'), \delta J(a, x'), \\ \delta J(a, z) .$$

Dependent parameter variations:

$$\delta U(x', \beta') = \delta U(x', \alpha') , \quad (\text{D.14})$$

$$\delta U(\alpha', \gamma) = \delta U(a, \alpha') + \frac{3}{5}\delta U(x', \gamma) + \frac{2}{5}\delta U(z, \gamma) ,$$

$$\delta J(a, \alpha') = -\frac{25}{372}\delta U(z) + \frac{73}{372}\delta U(\alpha') + \frac{175}{372}\delta U(x', y') \\ -\frac{1}{16\sqrt{15}}\delta U(a, \alpha') - \frac{85}{186}\delta U(x', \alpha') + \frac{5}{186}\delta U(a, \gamma) \\ +\frac{5}{31}\delta U(z, \alpha') - \frac{4}{93}\delta U(x', \gamma) + \frac{1}{16\sqrt{15}}\delta U(z, \gamma) \\ -\frac{5}{124}\delta U(\alpha', \beta') + \frac{20}{93}\delta J(x', \alpha') + \frac{265}{279}\delta J(a, x') \\ +\frac{25}{93}\delta J(a, z) ,$$

$$\delta J(a, \gamma) = \frac{1}{4}\delta U(\gamma) - \frac{1}{2}\delta U(a, \gamma) ,$$

$$\delta J(x', y') = -\frac{1}{2}\delta U(x', y') ,$$

$$\delta J(x', z) = \frac{211}{744}\delta U(z) + \frac{5}{186}\delta U(\alpha') - \frac{175}{744}\delta U(x', y') \\ -\frac{1}{2}\delta U(x', z) - \frac{15}{62}\delta U(a, \alpha') + \frac{85}{372}\delta U(x', \alpha') \\ -\frac{5}{372}\delta U(a, \gamma) - \frac{5}{62}\delta U(z, \alpha') + \frac{2}{93}\delta U(x', \gamma) \\ -\frac{1}{32\sqrt{15}}\delta U(z, \gamma) + \frac{5}{248}\delta U(\alpha', \beta') - \frac{10}{93}\delta J(x', \alpha') \\ +\frac{100}{279}\delta J(a, x') - \frac{25}{186}\delta J(a, z) ,$$

$$\delta J(y', \alpha') = \delta J(x', \alpha') ,$$

$$\delta J(z, \alpha') = \frac{25}{124}\delta U(z) - \frac{115}{248}\delta U(\alpha') + \frac{735}{248}\delta U(x', y') \\ +\frac{189}{62}\delta U(a, \alpha') - \frac{66}{31}\delta U(x', \alpha') + \frac{21}{124}\delta U(a, \gamma) \\ +\frac{16}{31}\delta U(z, \alpha') - \frac{42}{155}\delta U(x', \gamma) + \frac{63}{620}\delta U(z, \gamma) \\ -\frac{63}{248}\delta U(\alpha', \beta') + \frac{177}{62}\delta J(x', \alpha') - \frac{16}{31}\delta J(a, x') \\ +\frac{6}{31}\delta J(a, z) ,$$

$$\delta J(z, \gamma) = -\frac{5}{12}\delta U(\gamma) + \frac{8}{3}\delta J(x', \gamma) + \frac{4}{3}\delta U(x', \gamma) \\ -\frac{1}{2}\delta U(z, \gamma) - \frac{8}{3}\delta J(a, x') + \delta J(a, z) ,$$

$$\delta J(\alpha', \beta') = \frac{1}{2}\delta U(\alpha') - \frac{1}{2}\delta U(\alpha', \beta') ,$$

$$\delta J(\alpha', \gamma) = -\frac{25}{372}\delta U(z) + \frac{73}{372}\delta U(\alpha') - \frac{1}{6}\delta U(\gamma) \\ +\frac{175}{372}\delta U(x', y') - \frac{1}{16\sqrt{15}}\delta U(a, \alpha') - \frac{85}{186}\delta U(x', \alpha') \\ +\frac{5}{186}\delta U(a, \gamma) + \frac{5}{3}\delta J(x', \gamma) + \frac{5}{31}\delta U(z, \alpha')$$

$$+\frac{76}{155}\delta U(x', \gamma) - \frac{57}{310}\delta U(z, \gamma) - \frac{5}{124}\delta U(\alpha', \beta') \\ +\frac{20}{93}\delta J(x', \alpha') - \frac{200}{279}\delta J(a, x') + \frac{25}{93}\delta J(a, z) ,$$

$$\delta T(a; x', \alpha') = -\frac{5\sqrt{\frac{5}{3}}}{186}\delta U(z) + \frac{77\sqrt{\frac{5}{3}}}{744}\delta U(\alpha')$$

$$-\frac{37\sqrt{15}}{124}\delta U(x', y') - \frac{343}{62\sqrt{15}}\delta U(a, \alpha')$$

$$+\frac{211\sqrt{\frac{5}{3}}}{372}\delta U(x', \alpha') + \frac{4\sqrt{\frac{3}{5}}}{31}\delta U(a, \gamma) + \frac{2\sqrt{\frac{5}{3}}}{31}\delta U(z, \alpha')$$

$$-\frac{32\sqrt{\frac{3}{5}}}{155}\delta U(x', \gamma) + \frac{12\sqrt{\frac{3}{5}}}{155}\delta U(z, \gamma)$$

$$+\frac{83}{124\sqrt{15}}\delta U(\alpha', \beta') - \frac{77\sqrt{\frac{5}{3}}}{186}\delta J(x', \alpha')$$

$$-\frac{80\sqrt{\frac{5}{3}}}{279}\delta J(a, x') + \frac{10\sqrt{\frac{5}{3}}}{93}\delta J(a, z) ,$$

$$\delta T(x'; y', \beta') = \frac{8\sqrt{\frac{5}{3}}}{93}\delta U(z) + \frac{7\sqrt{\frac{5}{3}}}{372}\delta U(\alpha')$$

$$-\frac{56\sqrt{\frac{5}{3}}}{93}\delta U(x', y') - \frac{32\sqrt{\frac{3}{5}}}{31}\delta U(a, \alpha')$$

$$+\frac{637}{186\sqrt{15}}\delta U(x', \alpha') - \frac{16}{93\sqrt{15}}\delta U(a, \gamma)$$

$$-\frac{32}{31\sqrt{15}}\delta U(z, \alpha') + \frac{128}{465\sqrt{15}}\delta U(x', \gamma)$$

$$-\frac{16}{155\sqrt{15}}\delta U(z, \gamma) + \frac{8}{31\sqrt{15}}\delta U(\alpha', \beta')$$

$$-\frac{7\sqrt{\frac{5}{3}}}{93}\delta J(x', \alpha') + \frac{256\sqrt{\frac{5}{3}}}{279}\delta J(a, x')$$

$$-\frac{32\sqrt{\frac{5}{3}}}{93}\delta J(a, z) ,$$

$$\delta T(x'; z, \gamma) = \frac{113\sqrt{\frac{5}{3}}}{744}\delta U(z) - \frac{863}{1488\sqrt{15}}\delta U(\alpha')$$

$$+\frac{1}{\sqrt{15}}\delta U(\gamma) + \frac{253\sqrt{\frac{5}{3}}}{248}\delta U(x', y') - \frac{\sqrt{\frac{5}{3}}}{4}\delta U(x', z)$$

$$+\frac{73\sqrt{\frac{3}{5}}}{62}\delta U(a, \alpha') - \frac{529}{744\sqrt{15}}\delta U(x', \alpha')$$

$$+\frac{19}{31\sqrt{15}}\delta U(a, \gamma) - \frac{4}{\sqrt{15}}\delta J(x', \gamma)$$

$$-\frac{133}{124\sqrt{15}}\delta U(z, \alpha') - \frac{309\sqrt{\frac{3}{5}}}{155}\delta U(x', \gamma)$$

$$+\frac{174\sqrt{\frac{3}{5}}}{155}\delta U(z, \gamma) - \frac{73}{248\sqrt{15}}\delta U(\alpha', \beta')$$

$$\begin{aligned}
& + \frac{863}{372\sqrt{15}}\delta J(x', \alpha') + \frac{452\sqrt{\frac{5}{3}}}{279}\delta J(a, x') \\
& - \frac{113\sqrt{\frac{5}{3}}}{186}\delta J(a, z) ,
\end{aligned}$$

$$\begin{aligned}
\delta T(\gamma; x', \alpha') &= \frac{5\sqrt{\frac{5}{3}}}{186}\delta U(z) - \frac{77\sqrt{\frac{5}{3}}}{744}\delta U(\alpha') \\
& + \frac{37\sqrt{15}}{124}\delta U(x', y') + \frac{343}{62\sqrt{15}}\delta U(a, \alpha') \\
& - \frac{211\sqrt{\frac{5}{3}}}{372}\delta U(x', \alpha') - \frac{4\sqrt{\frac{3}{5}}}{31}\delta U(a, \gamma) \\
& - \frac{2\sqrt{\frac{5}{3}}}{31}\delta U(z, \alpha') - \frac{123\sqrt{\frac{3}{5}}}{155}\delta U(x', \gamma) \\
& + \frac{143\sqrt{\frac{3}{5}}}{155}\delta U(z, \gamma) - \frac{83}{124\sqrt{15}}\delta U(\alpha', \beta') \\
& + \frac{77\sqrt{\frac{5}{3}}}{186}\delta J(x', \alpha') + \frac{80\sqrt{\frac{5}{3}}}{279}\delta J(a, x') \\
& - \frac{10\sqrt{\frac{5}{3}}}{93}\delta J(a, z) ,
\end{aligned}$$

$$\begin{aligned}
\delta A(a; a, \alpha') &= \frac{5\sqrt{15}}{248}\delta U(z) - \frac{19\sqrt{\frac{5}{3}}}{248}\delta U(\alpha') \\
& + \frac{11\sqrt{\frac{5}{3}}}{93}\delta U(x', y') + \frac{133}{124\sqrt{15}}\delta U(a, \alpha') \\
& + \frac{5\sqrt{\frac{5}{3}}}{31}\delta U(x', \alpha') - \frac{107}{372\sqrt{15}}\delta U(a, \gamma) \\
& - \frac{3\sqrt{15}}{62}\delta U(z, \alpha') + \frac{214}{465\sqrt{15}}\delta U(x', \gamma) \\
& - \frac{107}{620\sqrt{15}}\delta U(z, \gamma) - \frac{2\sqrt{\frac{3}{5}}}{31}\delta U(\alpha', \beta') \\
& + \frac{19\sqrt{\frac{5}{3}}}{62}\delta J(x', \alpha') - \frac{11\sqrt{\frac{5}{3}}}{31}\delta J(a, x') \\
& - \frac{5\sqrt{15}}{62}\delta J(a, z) ,
\end{aligned}$$

$$\begin{aligned}
\delta A(x'; x', \alpha') &= \frac{8\sqrt{\frac{5}{3}}}{93}\delta U(z) + \frac{7\sqrt{\frac{5}{3}}}{372}\delta U(\alpha') \\
& - \frac{56\sqrt{\frac{5}{3}}}{93}\delta U(x', y') - \frac{32\sqrt{\frac{3}{5}}}{31}\delta U(a, \alpha') \\
& + \frac{637}{186\sqrt{15}}\delta U(x', \alpha') - \frac{16}{93\sqrt{15}}\delta U(a, \gamma) \\
& - \frac{32}{31\sqrt{15}}\delta U(z, \alpha') + \frac{128}{465\sqrt{15}}\delta U(x', \gamma) \\
& - \frac{16}{155\sqrt{15}}\delta U(z, \gamma) + \frac{8}{31\sqrt{15}}\delta U(\alpha', \beta')
\end{aligned}$$

$$\begin{aligned}
& - \frac{7\sqrt{\frac{5}{3}}}{93}\delta J(x', \alpha') + \frac{256\sqrt{\frac{5}{3}}}{279}\delta J(a, x') \\
& - \frac{32\sqrt{\frac{5}{3}}}{93}\delta J(a, z) ,
\end{aligned}$$

$$\begin{aligned}
\delta A(x'; x', \gamma) &= -\frac{29\sqrt{\frac{5}{3}}}{2976}\delta U(z) + \frac{1279}{2976\sqrt{15}}\delta U(\alpha') \\
& - \frac{1}{4\sqrt{15}}\delta U(\gamma) - \frac{1123\sqrt{\frac{5}{3}}}{1488}\delta U(x', y') + \frac{\sqrt{\frac{5}{3}}}{8}\delta U(x', z) \\
& - \frac{25\sqrt{15}}{124}\delta U(a, \alpha') + \frac{2297}{1488\sqrt{15}}\delta U(x', \alpha') \\
& - \frac{7\sqrt{\frac{5}{3}}}{93}\delta U(a, \gamma) + \frac{1}{\sqrt{15}}\delta J(x', \gamma) \\
& + \frac{29}{248\sqrt{15}}\delta U(z, \alpha') + \frac{242}{93\sqrt{15}}\delta U(x', \gamma) \\
& - \frac{107}{62\sqrt{15}}\delta U(z, \gamma) + \frac{25\sqrt{\frac{5}{3}}}{496}\delta U(\alpha', \beta') \\
& - \frac{1279}{744\sqrt{15}}\delta J(x', \alpha') - \frac{29\sqrt{\frac{5}{3}}}{279}\delta J(a, x') \\
& + \frac{29\sqrt{\frac{5}{3}}}{744}\delta J(a, z) ,
\end{aligned}$$

$$\begin{aligned}
\delta A(y'; x', \alpha') &= -\frac{8\sqrt{\frac{5}{3}}}{93}\delta U(z) - \frac{7\sqrt{\frac{5}{3}}}{372}\delta U(\alpha') \\
& + \frac{56\sqrt{\frac{5}{3}}}{93}\delta U(x', y') + \frac{32\sqrt{\frac{3}{5}}}{31}\delta U(a, \alpha') \\
& - \frac{637}{186\sqrt{15}}\delta U(x', \alpha') + \frac{16}{93\sqrt{15}}\delta U(a, \gamma) \\
& + \frac{32}{31\sqrt{15}}\delta U(z, \alpha') - \frac{128}{465\sqrt{15}}\delta U(x', \gamma) \\
& + \frac{16}{155\sqrt{15}}\delta U(z, \gamma) - \frac{8}{31\sqrt{15}}\delta U(\alpha', \beta') \\
& + \frac{7\sqrt{\frac{5}{3}}}{93}\delta J(x', \alpha') - \frac{256\sqrt{\frac{5}{3}}}{279}\delta J(a, x') \\
& + \frac{32\sqrt{\frac{5}{3}}}{93}\delta J(a, z) ,
\end{aligned}$$

$$\begin{aligned}
\delta A(\gamma; x', \alpha') &= -\frac{5\sqrt{15}}{248}\delta U(z) + \frac{19\sqrt{\frac{5}{3}}}{248}\delta U(\alpha') \\
& - \frac{\sqrt{\frac{5}{3}}}{4}\delta U(\gamma) - \frac{11\sqrt{\frac{5}{3}}}{93}\delta U(x', y') - \frac{133}{124\sqrt{15}}\delta U(a, \alpha') \\
& - \frac{5\sqrt{\frac{5}{3}}}{31}\delta U(x', \alpha') + \frac{107}{372\sqrt{15}}\delta U(a, \gamma) + \sqrt{\frac{5}{3}}\delta J(x', \gamma)
\end{aligned}$$

$$\begin{aligned}
& + \frac{3\sqrt{15}}{62}\delta U(z, \alpha') + \frac{1646}{465\sqrt{15}}\delta U(x', \gamma) \\
& - \frac{823}{620\sqrt{15}}\delta U(z, \gamma) + \frac{2\sqrt{\frac{3}{5}}}{31}\delta U(\alpha', \beta') \\
& - \frac{19\sqrt{\frac{5}{3}}}{62}\delta J(x', \alpha') - \frac{20\sqrt{\frac{5}{3}}}{31}\delta J(a, x') \\
& + \frac{5\sqrt{15}}{62}\delta J(a, z), \\
\delta S(a, x'; y', z) &= \frac{113\sqrt{\frac{5}{3}}}{744}\delta U(z) - \frac{863}{1488\sqrt{15}}\delta U(\alpha') \\
& + \frac{253\sqrt{\frac{5}{3}}}{248}\delta U(x', y') - \frac{\sqrt{\frac{5}{3}}}{4}\delta U(x', z) + \frac{73\sqrt{\frac{3}{5}}}{62}\delta U(a, \alpha') \\
& - \frac{529}{744\sqrt{15}}\delta U(x', \alpha') + \frac{19}{31\sqrt{15}}\delta U(a, \gamma) \\
& - \frac{133}{124\sqrt{15}}\delta U(z, \alpha') - \frac{152}{155\sqrt{15}}\delta U(x', \gamma) \\
& + \frac{19\sqrt{\frac{3}{5}}}{155}\delta U(z, \gamma) - \frac{73}{248\sqrt{15}}\delta U(\alpha', \beta') \\
& + \frac{863}{372\sqrt{15}}\delta J(x', \alpha') + \frac{1144}{279\sqrt{15}}\delta J(a, x') \\
& - \frac{113\sqrt{\frac{5}{3}}}{186}\delta J(a, z), \\
\delta S(a, x'; z, y') &= -\frac{29\sqrt{\frac{5}{3}}}{2976}\delta U(z) + \frac{1279}{2976\sqrt{15}}\delta U(\alpha') \\
& - \frac{1123\sqrt{\frac{5}{3}}}{1488}\delta U(x', y') + \frac{\sqrt{\frac{5}{3}}}{8}\delta U(x', z) \\
& - \frac{25\sqrt{15}}{124}\delta U(a, \alpha') + \frac{2297}{1488\sqrt{15}}\delta U(x', \alpha') \\
& - \frac{7\sqrt{\frac{5}{3}}}{93}\delta U(a, \gamma) + \frac{29}{248\sqrt{15}}\delta U(z, \alpha') \\
& + \frac{56}{93\sqrt{15}}\delta U(x', \gamma) - \frac{7}{31\sqrt{15}}\delta U(z, \gamma) \\
& + \frac{25\sqrt{\frac{5}{3}}}{496}\delta U(\alpha', \beta') - \frac{1279}{744\sqrt{15}}\delta J(x', \alpha') \\
& + \frac{134}{279\sqrt{15}}\delta J(a, x') + \frac{29\sqrt{\frac{5}{3}}}{744}\delta J(a, z), \\
\delta S(a, x'; z, \beta') &= -\frac{425}{8928}\delta U(z) + \frac{101}{2232}\delta U(\alpha') \\
& - \frac{35}{1116}\delta U(x', y') - \frac{1}{31}\delta U(a, \alpha') - \frac{59}{1116}\delta U(x', \alpha') \\
& - \frac{1}{558}\delta U(a, \gamma) - \frac{\sqrt{15}}{360}\delta U(z, \alpha') + \frac{4}{1395}\delta U(x', \gamma) \\
& - \frac{1}{930}\delta U(z, \gamma) + \frac{1}{372}\delta U(\alpha', \beta') - \frac{101}{558}\delta J(x', \alpha')
\end{aligned}$$

$$\begin{aligned}
& - \frac{146}{837}\delta J(a, x') + \frac{425}{2232}\delta J(a, z), \\
\delta S(a, x'; \gamma, y') &= -\frac{15}{124}\delta U(z) + \frac{69}{248}\delta U(\alpha') - \frac{1}{8}\delta U(\gamma) \\
& - \frac{441}{248}\delta U(x', y') - \frac{567}{310}\delta U(a, \alpha') + \frac{21}{31}\delta U(x', \alpha') \\
& - \frac{63}{620}\delta U(a, \gamma) + \frac{1}{2}\delta J(x', \gamma) + \frac{9}{31}\delta U(z, \alpha') \\
& + \frac{1337}{1550}\delta U(x', \gamma) - \frac{396}{775}\delta U(z, \gamma) + \frac{189}{1240}\delta U(\alpha', \beta') \\
& - \frac{69}{62}\delta J(x', \alpha') - \frac{49}{62}\delta J(a, x') + \frac{15}{31}\delta J(a, z), \\
\delta S(a, x'; \gamma, \beta') &= -\frac{5\sqrt{15}}{248}\delta U(z) + \frac{19\sqrt{\frac{5}{3}}}{248}\delta U(\alpha') \\
& - \frac{\sqrt{\frac{5}{3}}}{8}\delta U(\gamma) - \frac{11\sqrt{\frac{5}{3}}}{93}\delta U(x', y') - \frac{133}{124\sqrt{15}}\delta U(a, \alpha'), \\
& - \frac{5\sqrt{\frac{5}{3}}}{31}\delta U(x', \alpha') + \frac{107}{372\sqrt{15}}\delta U(a, \gamma) + \frac{1}{2}\sqrt{\frac{5}{3}}\delta J(x', \gamma) \\
& + \frac{3\sqrt{15}}{62}\delta U(z, \alpha') + \frac{716}{465\sqrt{15}}\delta U(x', \gamma) \\
& - \frac{179}{310\sqrt{15}}\delta U(z, \gamma) + \frac{2\sqrt{\frac{3}{5}}}{31}\delta U(\alpha', \beta') \\
& - \frac{19\sqrt{\frac{5}{3}}}{62}\delta J(x', \alpha') - \frac{3\sqrt{15}}{62}\delta J(a, x') + \frac{5\sqrt{15}}{62}\delta J(a, z), \\
\delta S(a, y'; \alpha', z) &= \frac{49}{160\sqrt{15}}\delta U(z) - \frac{421}{8928}\delta U(\alpha') \\
& + \frac{505}{4464}\delta U(x', y') - \frac{1}{8}\delta U(x', z) + \frac{81}{620}\delta U(a, \alpha') \\
& + \frac{373}{4464}\delta U(x', \alpha') - \frac{251}{2790}\delta U(a, \gamma) - \frac{11}{744}\delta U(z, \alpha') \\
& + \frac{1004}{6975}\delta U(x', \gamma) - \frac{251}{4650}\delta U(z, \gamma) - \frac{391}{7440}\delta U(\alpha', \beta') \\
& + \frac{421}{2232}\delta J(x', \alpha') + \frac{148}{837}\delta J(a, x') - \frac{353}{1116}\delta J(a, z), \\
\delta S(a, y'; \alpha', \gamma) &= \frac{5\sqrt{\frac{5}{3}}}{186}\delta U(z) - \frac{77\sqrt{\frac{5}{3}}}{744}\delta U(\alpha') \\
& + \frac{37\sqrt{15}}{124}\delta U(x', y') + \frac{343}{62\sqrt{15}}\delta U(a, \alpha') \\
& - \frac{211\sqrt{\frac{5}{3}}}{372}\delta U(x', \alpha') - \frac{4\sqrt{\frac{3}{5}}}{31}\delta U(a, \gamma) - \frac{2\sqrt{\frac{5}{3}}}{31}\delta U(z, \alpha') \\
& - \frac{91\sqrt{\frac{3}{5}}}{310}\delta U(x', \gamma) + \frac{131\sqrt{\frac{3}{5}}}{310}\delta U(z, \gamma) \\
& - \frac{83}{124\sqrt{15}}\delta U(\alpha', \beta') + \frac{77\sqrt{\frac{5}{3}}}{186}\delta J(x', \alpha') \\
& + \frac{80\sqrt{\frac{5}{3}}}{279}\delta J(a, x') - \frac{10\sqrt{\frac{5}{3}}}{93}\delta J(a, z),
\end{aligned}$$

$$\begin{aligned}
\delta S(a, z; \alpha', y') &= \frac{1}{16\sqrt{15}}\delta U(z) - \frac{43}{992}\delta U(\alpha') \\
&- \frac{25}{496}\delta U(x', y') + \frac{1}{8}\delta U(x', z) - \frac{41}{620}\delta U(a, \alpha') \\
&+ \frac{11}{496}\delta U(x', \alpha') + \frac{29}{310}\delta U(a, \gamma) + \frac{9}{248}\delta U(z, \alpha') \\
&- \frac{116}{775}\delta U(x', \gamma) + \frac{87}{1550}\delta U(z, \gamma) + \frac{117}{2480}\delta U(\alpha', \beta') \\
&+ \frac{43}{248}\delta J(x', \alpha') + \frac{16}{93}\delta J(a, x') - \frac{2}{31}\delta J(a, z), \\
\delta S(a, \alpha'; \gamma, \beta') &= -\frac{25}{279}\delta U(z) + \frac{305}{2232}\delta U(\alpha') \\
&- \frac{5}{24}\delta U(\gamma) - \frac{925}{2232}\delta U(x', y') - \frac{42}{31}\delta U(a, \alpha') \\
&+ \frac{125}{558}\delta U(x', \alpha') + \frac{691}{1116}\delta U(a, \gamma) + \frac{5}{6}\delta J(x', \gamma) \\
&+ \frac{20}{93}\delta U(z, \alpha') + \frac{491}{2790}\delta U(x', \gamma) - \frac{176}{465}\delta U(z, \gamma) \\
&+ \frac{239}{744}\delta U(\alpha', \beta') - \frac{305}{558}\delta J(x', \alpha') - \frac{205}{1674}\delta J(a, x') \\
&+ \frac{100}{279}\delta J(a, z), \\
\delta S(a, \beta'; \gamma, x') &= -\frac{5\sqrt{15}}{248}\delta U(z) + \frac{19\sqrt{\frac{5}{3}}}{248}\delta U(\alpha') \\
&- \frac{\sqrt{\frac{5}{3}}}{8}\delta U(\gamma) - \frac{11\sqrt{\frac{5}{3}}}{93}\delta U(x', y') - \frac{133}{124\sqrt{15}}\delta U(a, \alpha') \\
&- \frac{5\sqrt{\frac{5}{3}}}{31}\delta U(x', \alpha') + \frac{107}{372\sqrt{15}}\delta U(a, \gamma) + \frac{1}{2}\sqrt{\frac{5}{3}}\delta J(x', \gamma) \\
&+ \frac{3\sqrt{15}}{62}\delta U(z, \alpha') + \frac{716}{465\sqrt{15}}\delta U(x', \gamma) \\
&- \frac{179}{310\sqrt{15}}\delta U(z, \gamma) + \frac{2\sqrt{\frac{3}{5}}}{31}\delta U(\alpha', \beta') \\
&- \frac{19\sqrt{\frac{5}{3}}}{62}\delta J(x', \alpha') - \frac{3\sqrt{15}}{62}\delta J(a, x') + \frac{5\sqrt{15}}{62}\delta J(a, z), \\
\delta S(x', y'; \alpha', \beta') &= \frac{10}{279}\delta U(z) - \frac{61}{1116}\delta U(\alpha') \\
&+ \frac{743}{1116}\delta U(x', y') + \frac{84}{155}\delta U(a, \alpha') - \frac{25}{279}\delta U(x', \alpha') \\
&+ \frac{352}{1395}\delta U(a, \gamma) - \frac{8}{93}\delta U(z, \alpha') - \frac{2816}{6975}\delta U(x', \gamma) \\
&+ \frac{352}{2325}\delta U(z, \gamma) - \frac{239}{1860}\delta U(\alpha', \beta') + \frac{61}{279}\delta J(x', \alpha') \\
&+ \frac{320}{837}\delta J(a, x') - \frac{40}{279}\delta J(a, z), \\
\delta S(x', y'; \beta', \alpha') &= -\frac{10}{279}\delta U(z) + \frac{61}{1116}\delta U(\alpha') \\
&- \frac{743}{1116}\delta U(x', y') - \frac{84}{155}\delta U(a, \alpha') + \frac{25}{279}\delta U(x', \alpha') \\
&- \frac{352}{1395}\delta U(a, \gamma) + \frac{8}{93}\delta U(z, \alpha') + \frac{2816}{6975}\delta U(x', \gamma)
\end{aligned}$$

$$\begin{aligned}
&- \frac{352}{2325}\delta U(z, \gamma) + \frac{239}{1860}\delta U(\alpha', \beta') - \frac{61}{279}\delta J(x', \alpha') \\
&- \frac{320}{837}\delta J(a, x') + \frac{40}{279}\delta J(a, z), \\
\delta S(x', z; \alpha', \gamma) &= -\frac{1}{16\sqrt{15}}\delta U(z) + \frac{43}{992}\delta U(\alpha') \\
&+ \frac{25}{496}\delta U(x', y') - \frac{1}{8}\delta U(x', z) + \frac{41}{620}\delta U(a, \alpha') \\
&- \frac{11}{496}\delta U(x', \alpha') - \frac{29}{310}\delta U(a, \gamma) - \frac{9}{248}\delta U(z, \alpha') \\
&- \frac{233}{1550}\delta U(x', \gamma) + \frac{189}{775}\delta U(z, \gamma) - \frac{117}{2480}\delta U(\alpha', \beta') \\
&- \frac{43}{248}\delta J(x', \alpha') - \frac{16}{93}\delta J(a, x') + \frac{2}{31}\delta J(a, z), \\
\delta S(x', z; \gamma, \alpha') &= -\frac{49}{160\sqrt{15}}\delta U(z) + \frac{421}{8928}\delta U(\alpha') \\
&- \frac{1}{6}\delta U(\gamma) - \frac{505}{4464}\delta U(x', y') + \frac{1}{8}\delta U(x', z) \\
&- \frac{81}{620}\delta U(a, \alpha') - \frac{373}{4464}\delta U(x', \alpha') + \frac{251}{2790}\delta U(a, \gamma) \\
&+ \frac{2}{3}\delta J(x', \gamma) + \frac{11}{744}\delta U(z, \alpha') + \frac{6827}{13950}\delta U(x', \gamma) \\
&- \frac{572}{2325}\delta U(z, \gamma) + \frac{391}{7440}\delta U(\alpha', \beta') - \frac{421}{2232}\delta J(x', \alpha') \\
&- \frac{706}{837}\delta J(a, x') + \frac{353}{1116}\delta J(a, z), \\
\delta S(x', \alpha'; \gamma, z) &= -\frac{425}{8928}\delta U(z) + \frac{101}{2232}\delta U(\alpha') \\
&- \frac{1}{12}\delta U(\gamma) - \frac{35}{1116}\delta U(x', y') - \frac{1}{31}\delta U(a, \alpha') \\
&- \frac{59}{1116}\delta U(x', \alpha') - \frac{1}{558}\delta U(a, \gamma) + \frac{1}{3}\delta J(x', \gamma) \\
&- \frac{\sqrt{15}}{360}\delta U(z, \alpha') + \frac{473}{2790}\delta U(x', \gamma) - \frac{1}{930}\delta U(z, \gamma) \\
&+ \frac{1}{372}\delta U(\alpha', \beta') - \frac{101}{558}\delta J(x', \alpha') - \frac{425}{837}\delta J(a, x') \\
&+ \frac{425}{2232}\delta J(a, z).
\end{aligned}$$

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